IPMU Focus Week on Quantum Mechanical Systems at Large Quantum Number

Bulk-boundary correspondence of topologically trivial insulators

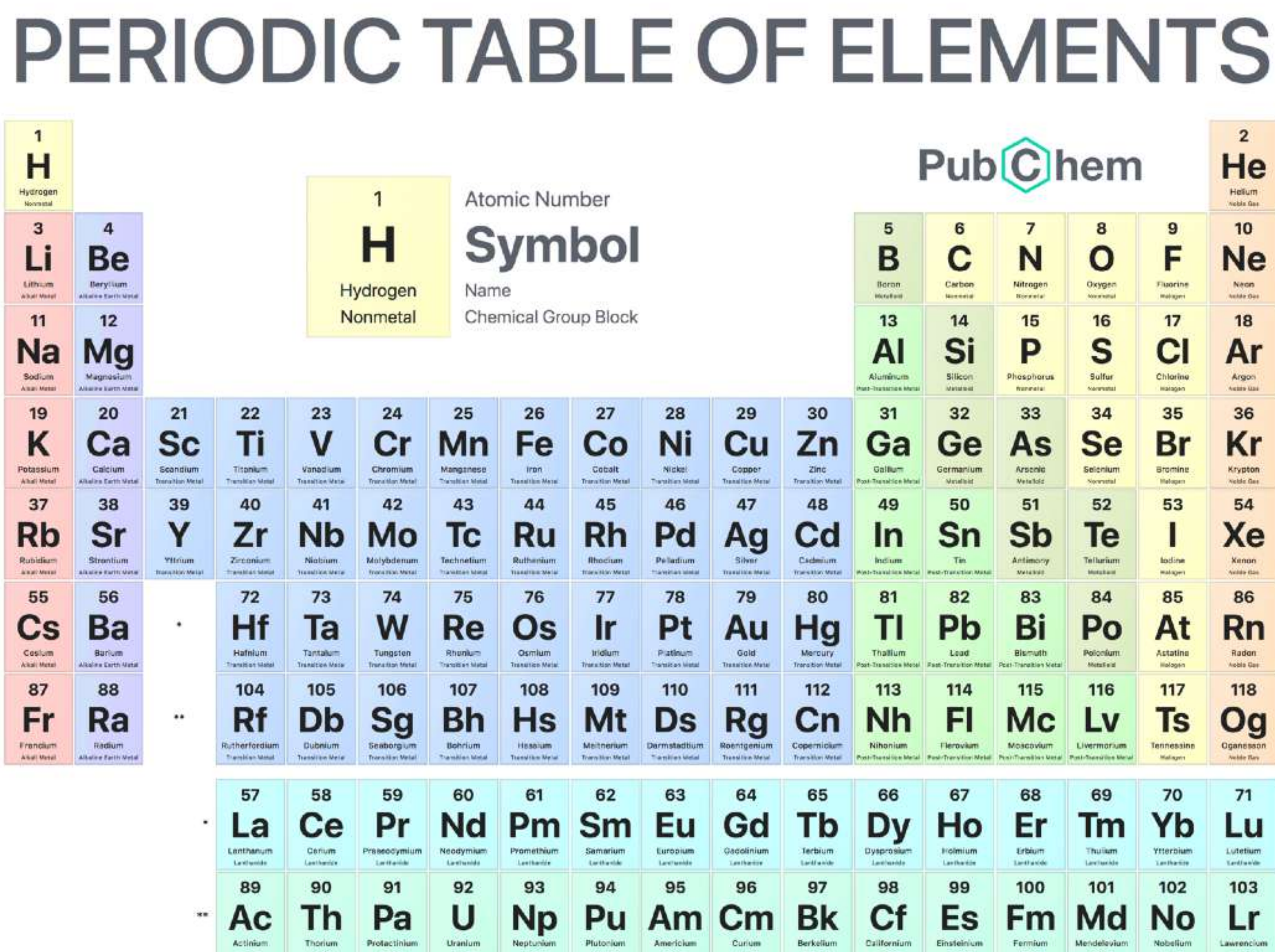
Haruki Watanabe
University of Tokyo

HW and S. Ono, Phys. Rev. B 102, 165120 (2020)
HW and H. C. Po, arXiv:2009.04845

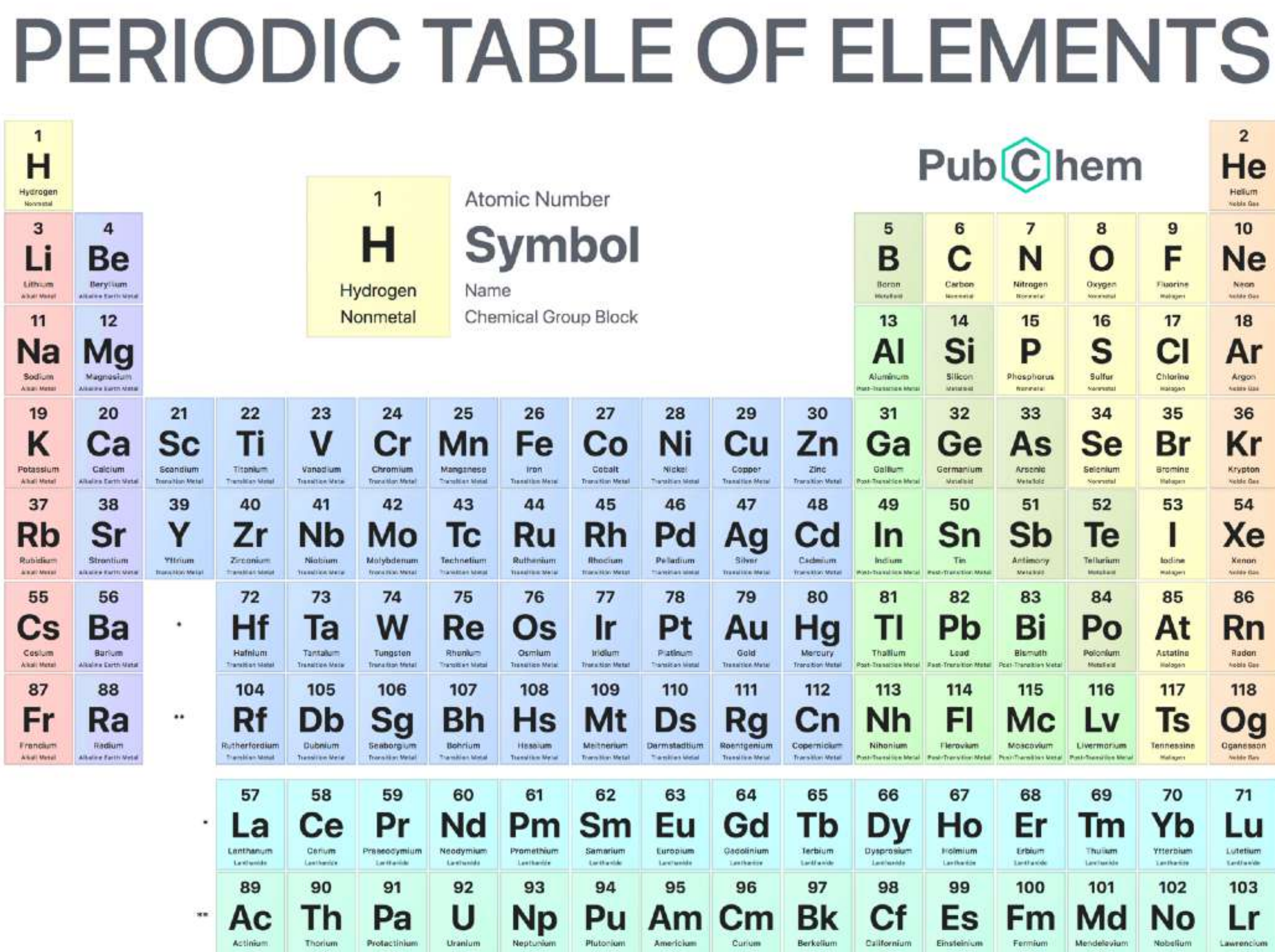
Seishiro Ono
The University of Tokyo

Hoi Chun Po
The Hong Kong University of Science and Technology

Variety of condensed matter

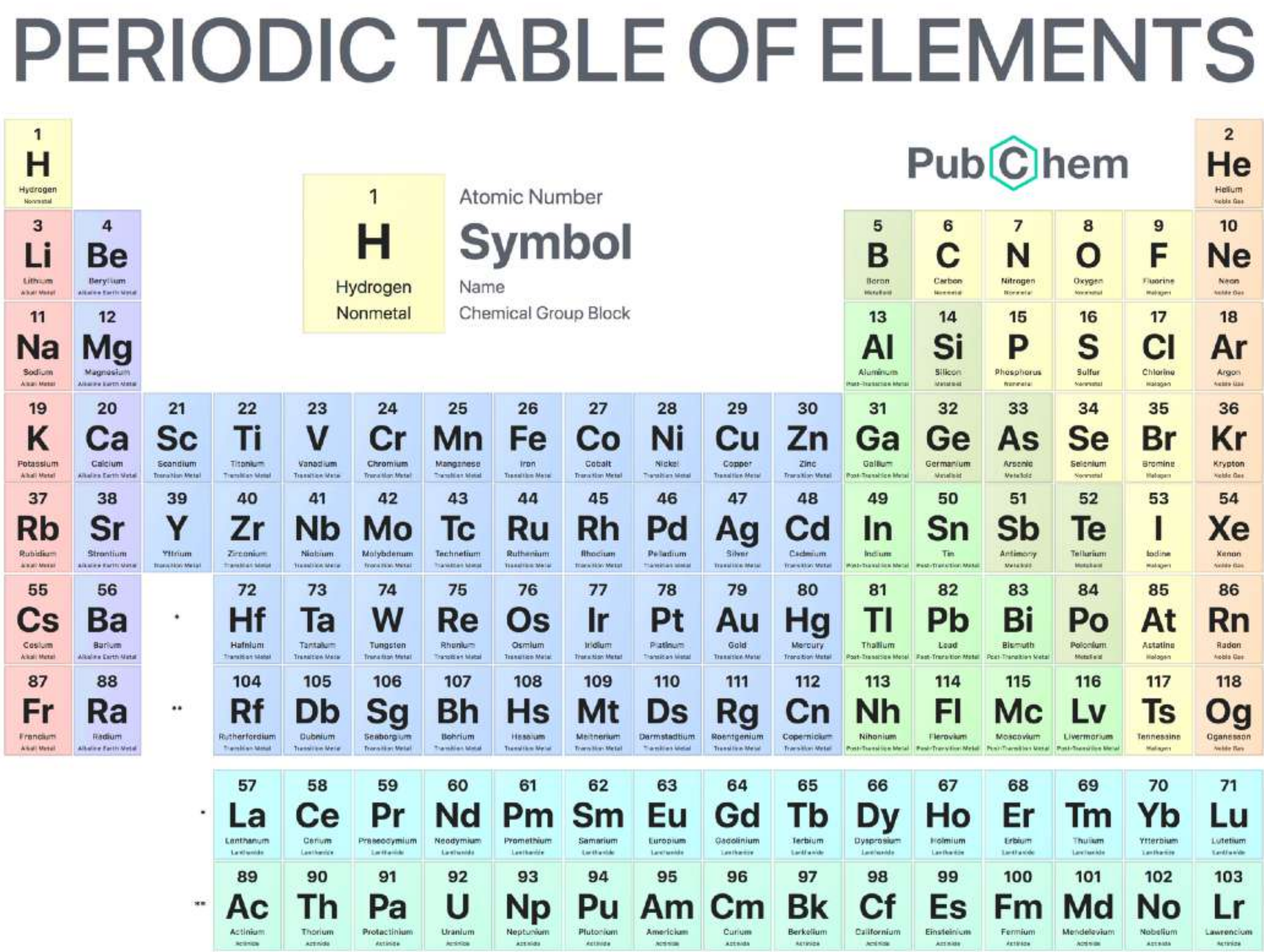


Variety of condensed matter



“Quantum Mechanical Systems”
at “Large Quantum Number”

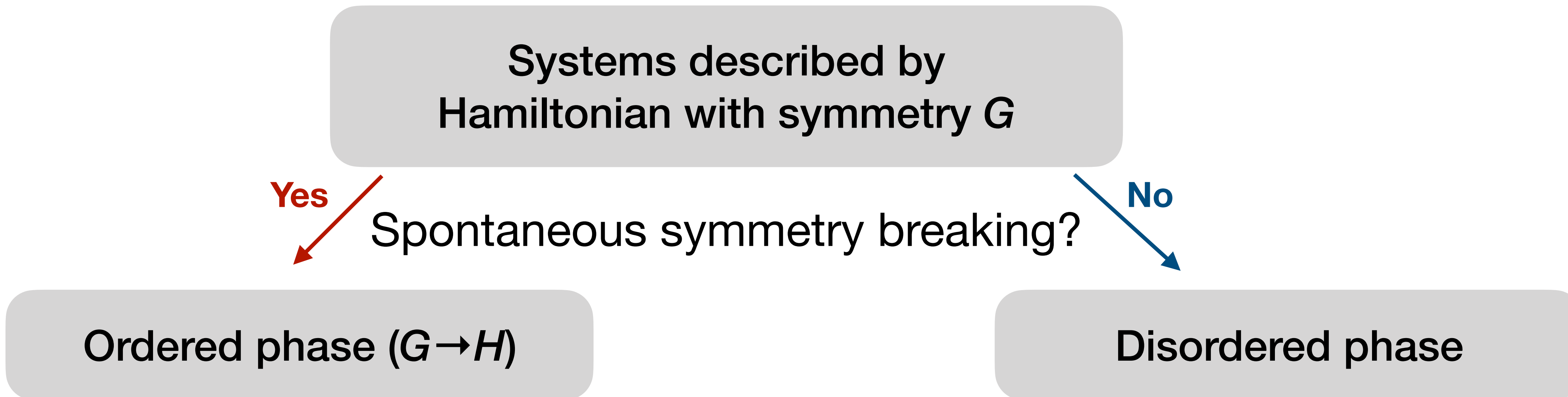
Variety of condensed matter



"Quantum Mechanical Systems"
at "Large Quantum Number"

(The topic today is unfortunately
not really quantum or with large quantum number)

Classification of *T*=0 phases



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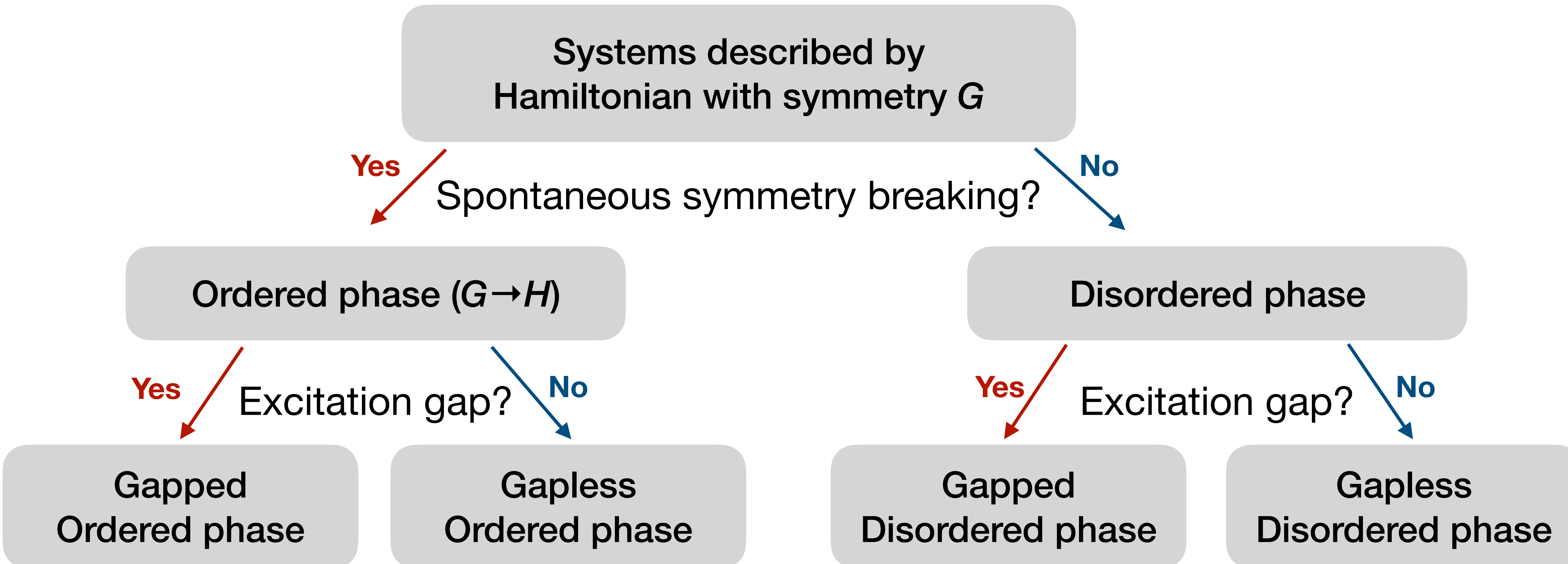
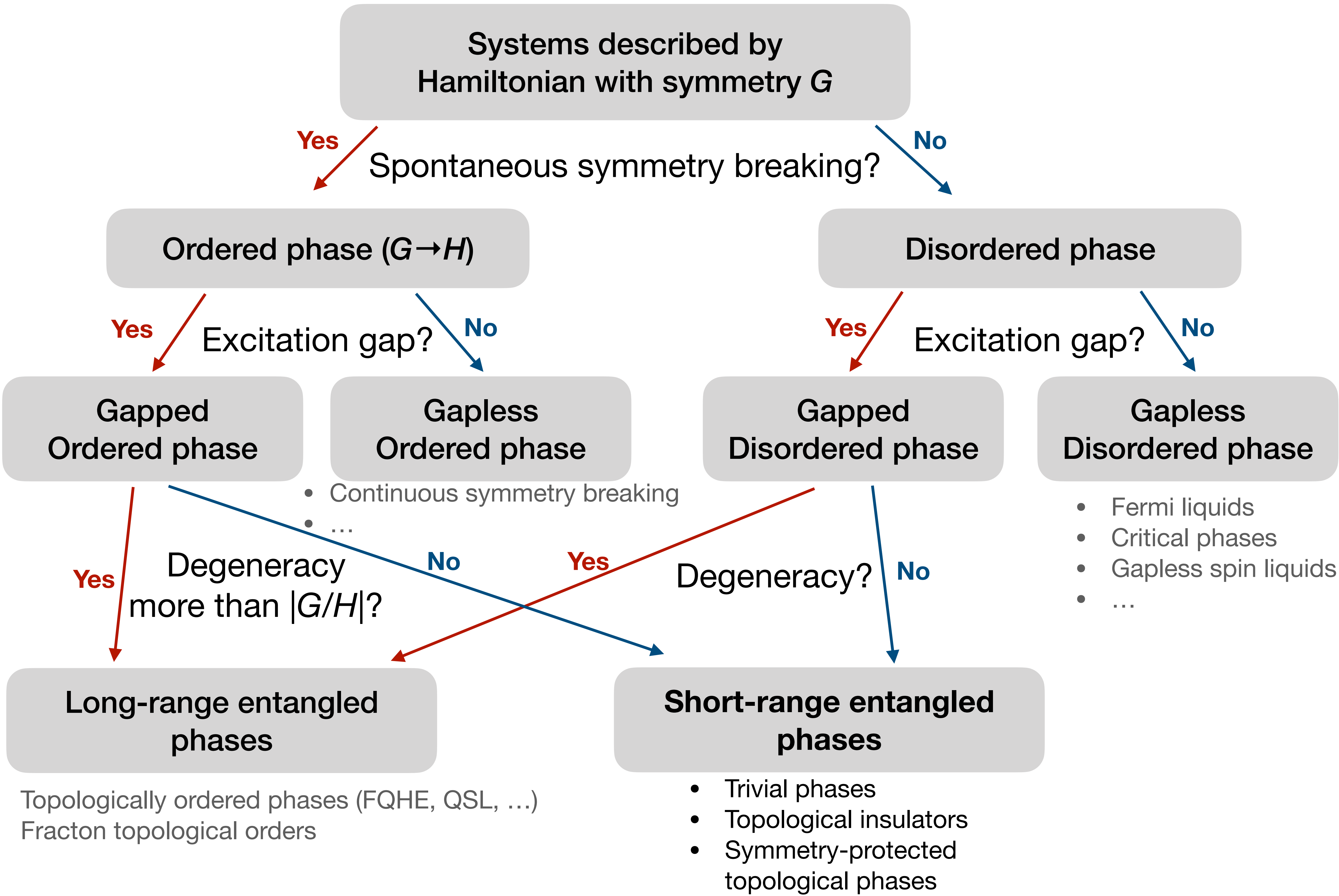


Classification of T=0 phases

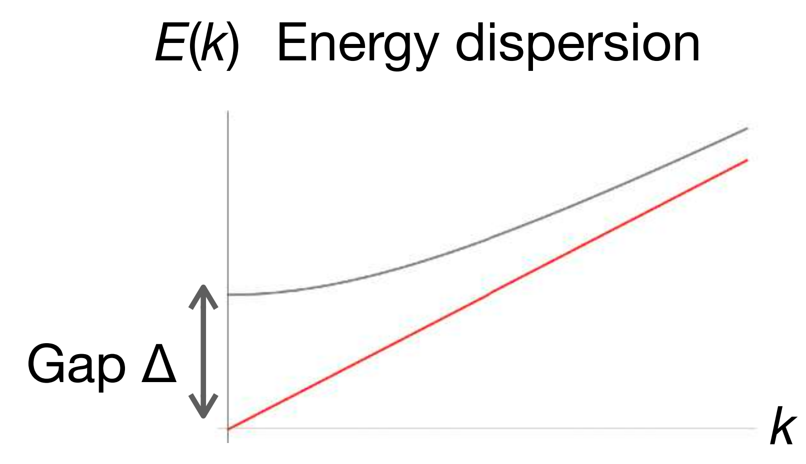


Nambu-Goldstone modes in relativistic systems

Upon spontaneous breaking of *G* into *H*

Counting rule: $n_{\mathrm{NGM}} = n_{\mathrm{BG}}$

$$n_{\mathrm{BG}} \equiv \dim G/H = \dim G - \dim H$$



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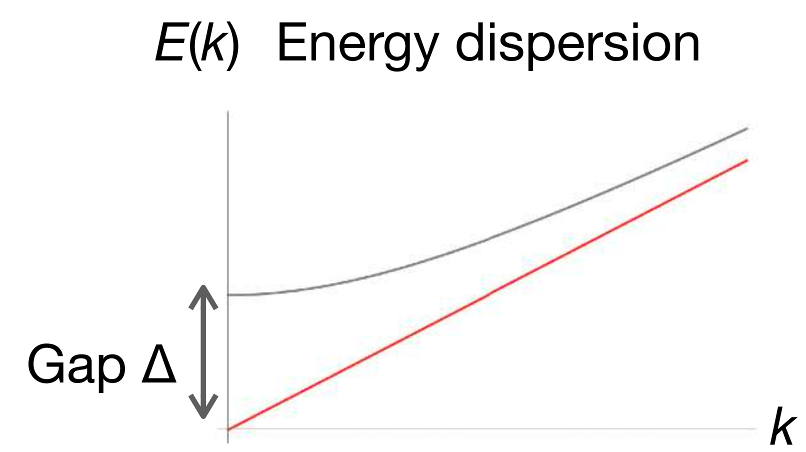
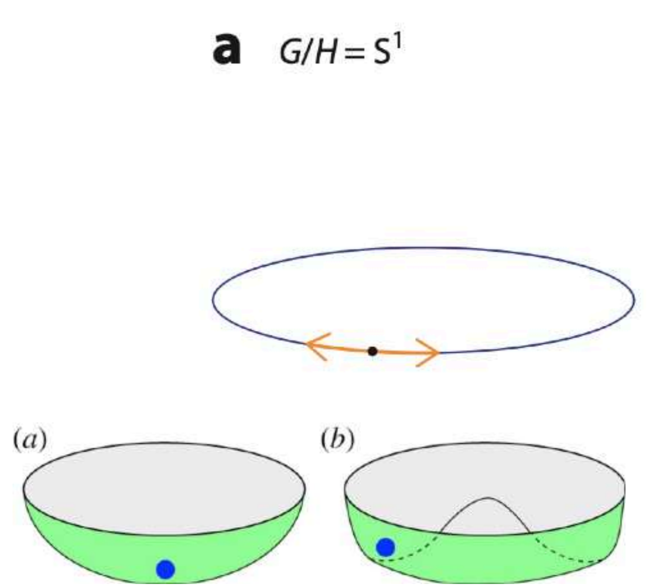


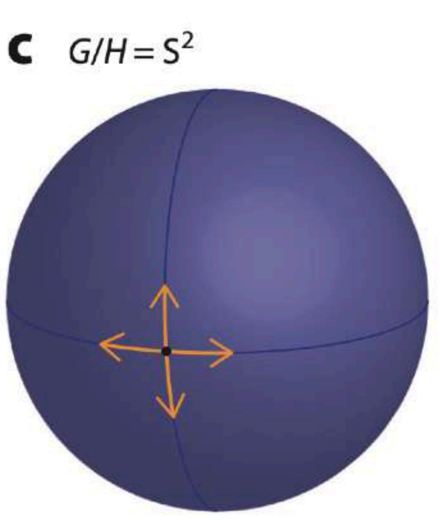
low-E effective Lagrangian

$$\mathcal{L}_{\mathrm{eff}} = \sum_{a,b} \sum_{\mu,\nu} \frac{1}{2} g_{ab}\, \eta^{\mu\nu} \omega^a_\mu \omega^b_\nu + \ldots,$$

Maurer–Cartan one-form

$$\sum_i \omega^i_\mu T_i \equiv -iU^\dagger \partial_\mu U, \quad U(\pi) \equiv e^{i\sum_a \pi^a T_a}.$$

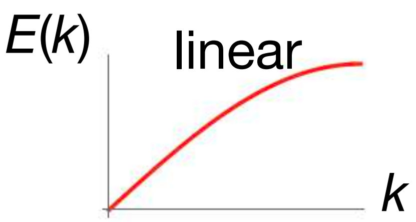


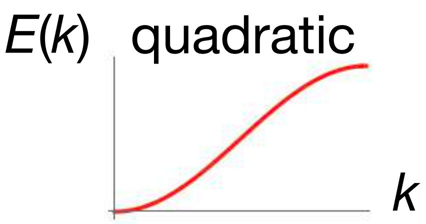


Nambu-Goldstone modes in *non-relativistic* systems

HW, H. Murayama, PRL (2012), HW, Annual Review of Condensed Matter Physics (2020)

$$n_{\text{NGM}} = n_{\text{BG}} - \frac{1}{2}\text{rank}\rho \qquad \rho_{ij} \equiv -i\frac{1}{V}\langle[\hat{Q}_i, \hat{Q}_j]\rangle = \sum_k f_{ij}{}^k \frac{\langle\hat{Q}_k\rangle}{V}$$





$$\rho = \left(\begin{array}{cccccccc|c} 0 & \lambda_1 & & & & & & & \\ -\lambda_1 & 0 & & & & & & & \\ & & 0 & \lambda_2 & & & & & \\ & & -\lambda_2 & 0 & & & & & \\ & & & & \ddots & & & & \\ & & & & & & 0 & \lambda_m & \\ & & & & & & -\lambda_m & 0 & \\ \hline & & & & & & & & O \end{array}\right)$$

Nambu-Goldstone modes in *non-relativistic* systems

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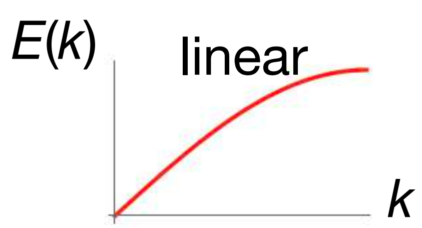

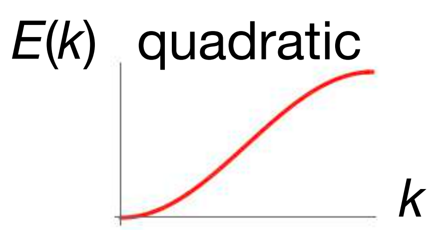

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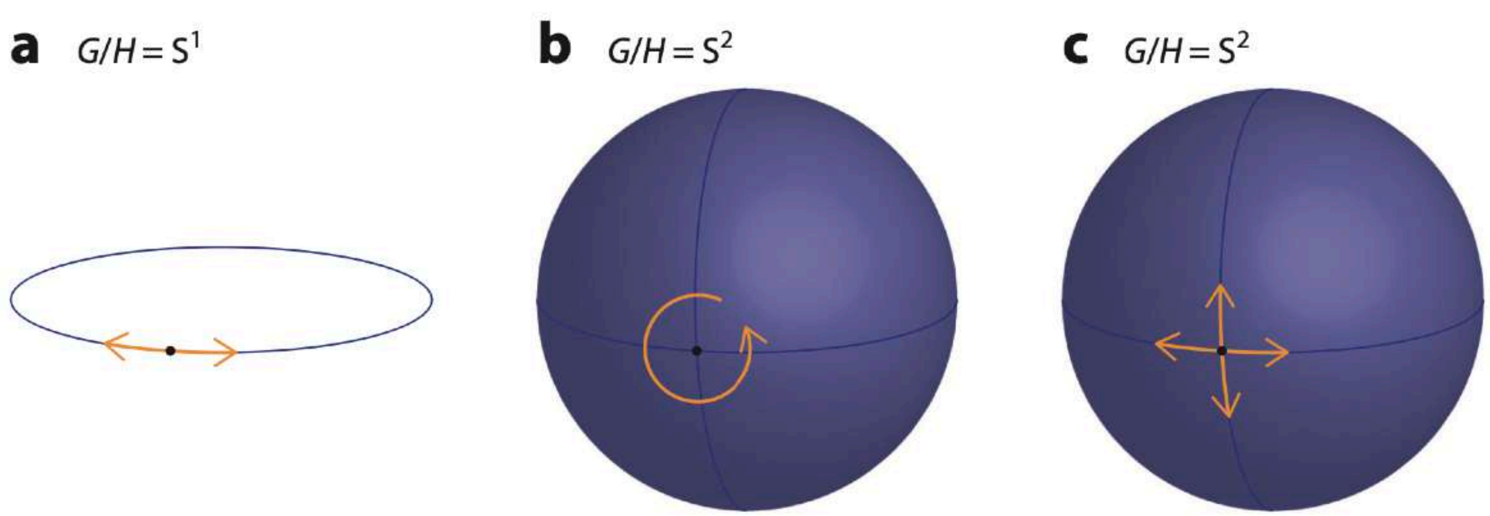
$$\mathcal{L}_{\rm eff} = -\sum_i e_i\,\omega_t^i + \sum_{a,b}\frac{1}{2}\bar{g}_{ab}\,\omega_t^a\omega_t^b - \sum_{a,b}\sum_{r=x,y,z}\frac{1}{2}g_{ab}\,\omega_r^a\omega_r^b + \ldots.$$

$$\simeq \sum_{a,b}\frac{1}{2}\rho_{ab}\,\partial_t\pi^a\pi^b + \sum_{a,b}\frac{1}{2}\bar{g}_{ab}\,\partial_t\pi^a\partial_t\pi^b - \sum_{a,b}\sum_{r=x,y,z}\frac{1}{2}g_{ab}\,\partial_r\pi^a\partial_r\pi^b + \ldots.$$

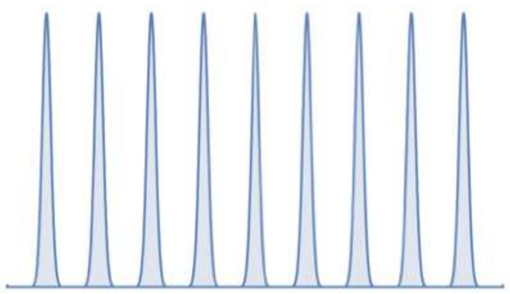


Quantum Time Crystals

F. Wilczek. PRL (2012)

(conventional) crystal

<ρ(x)> : ground-state expectation
value of density of ions, atoms, …



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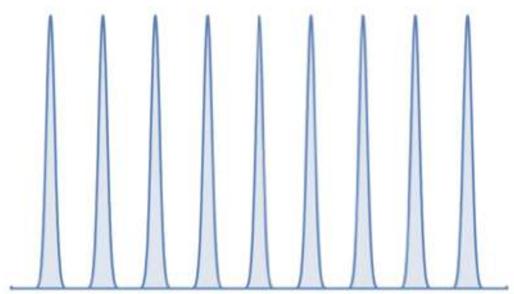
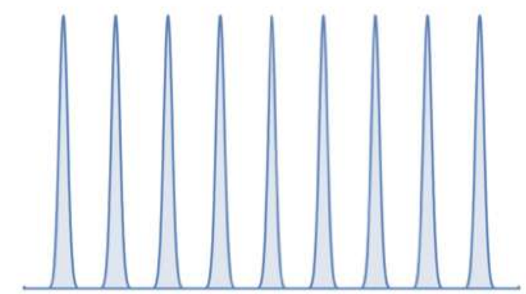


position x

Quantum Time Crystal

<O(t)> : ground-state expectation value of an observable



time t

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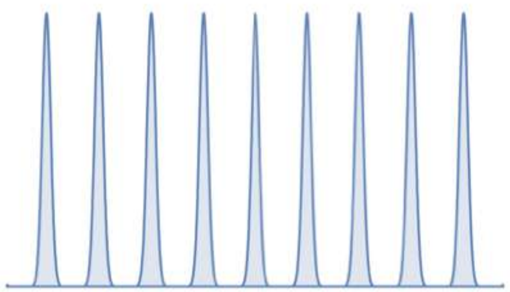

$$\lim_{V\to\infty}\langle\hat{\phi}(\vec{x},0)\hat{\phi}(\vec{x}',0)\rangle \to f(\vec{x}-\vec{x}')$$

Quantum Time Crystal

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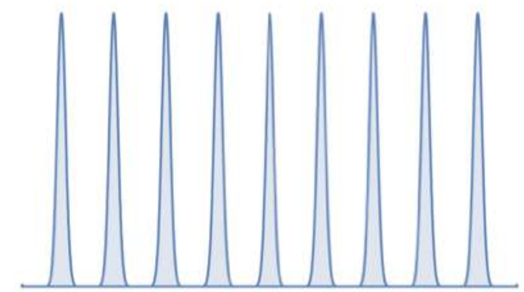
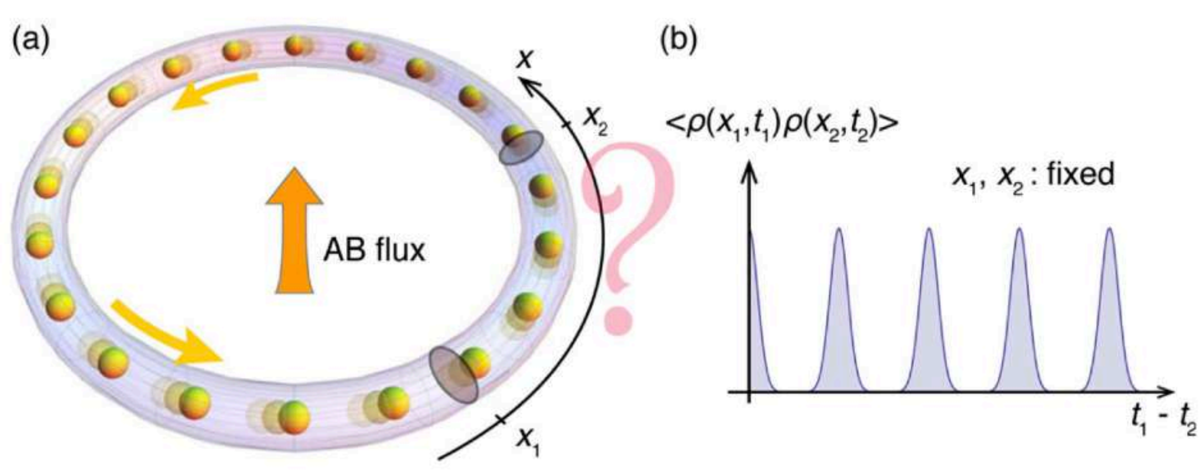
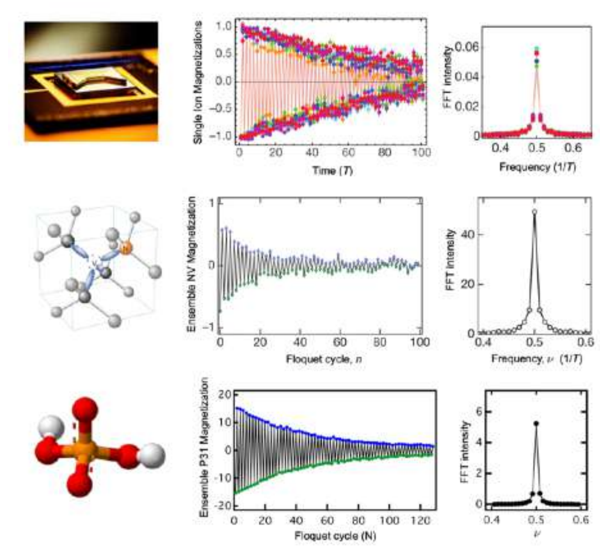


$$\lim_{V\to\infty}\langle\hat{\phi}(\vec{x},t)\hat{\phi}(0,0)\rangle \to f(t)$$





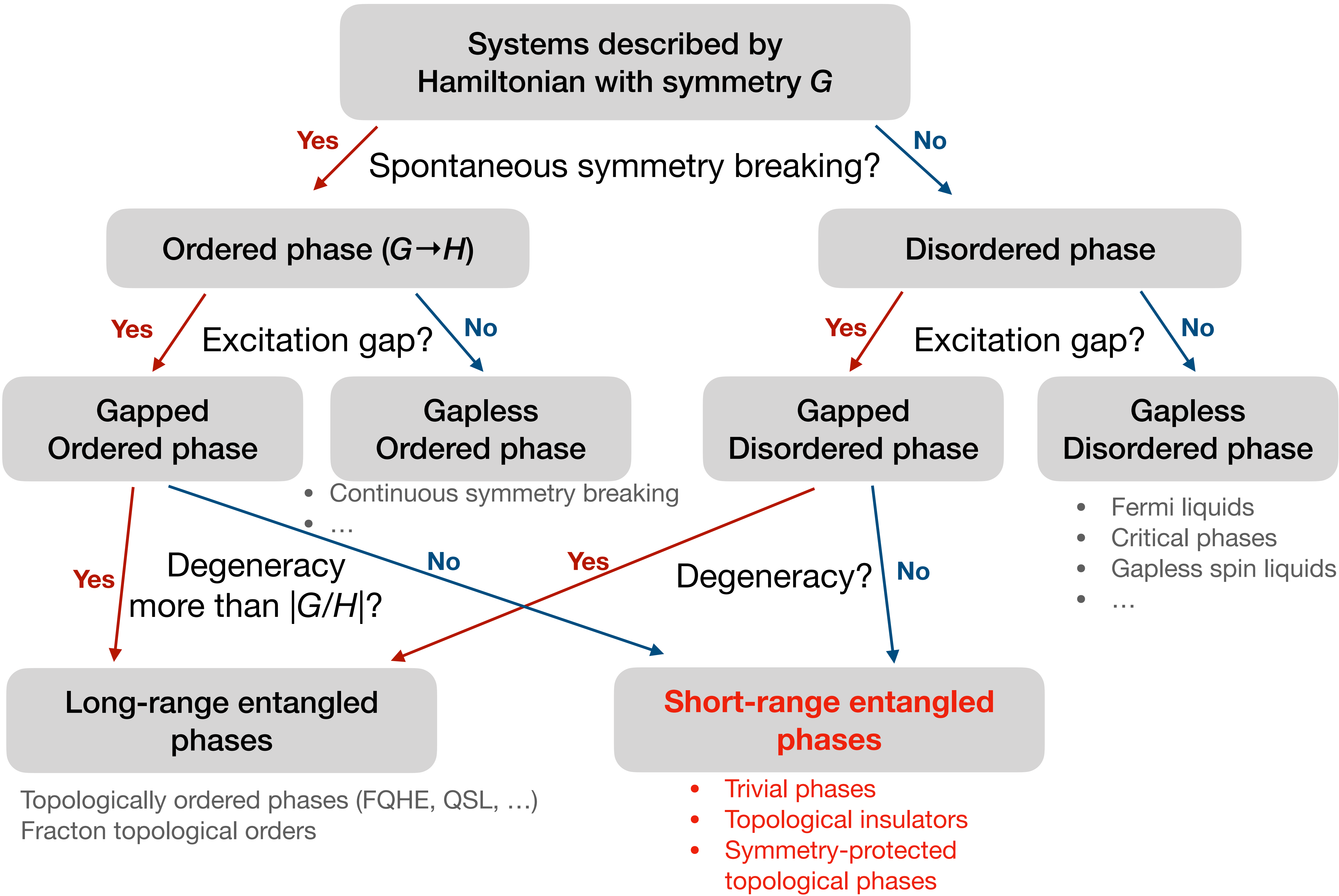
We showed f(t) is time-independent → absence of QTC

HW, M. Oshikawa, PRL (2015)

→ Recent realization of Discrete Time Crystals (in driven systems)

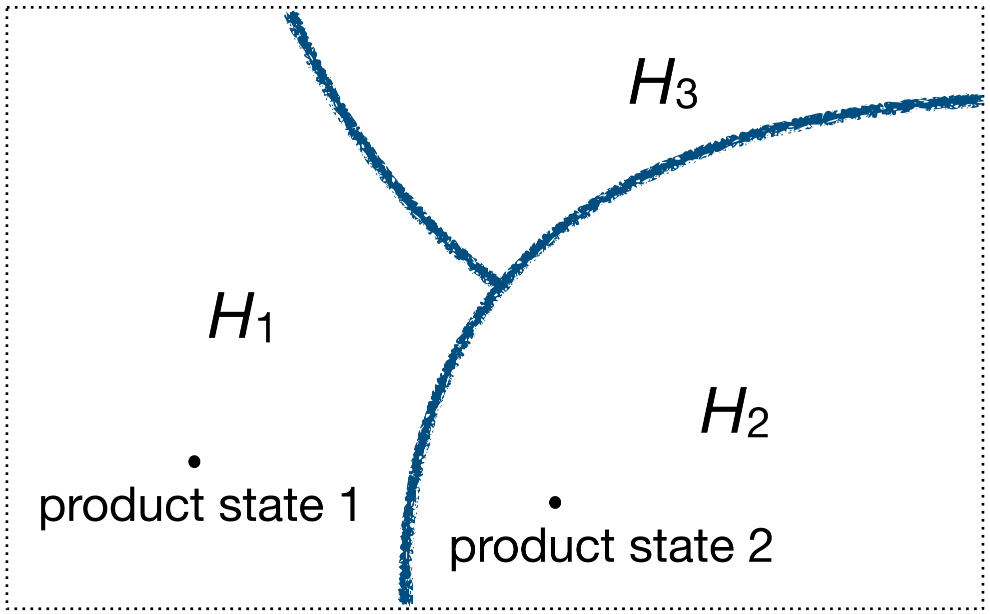
D. V. Else, et al, ARCMP (2020)

Classification of T=0 phases



Classification of short-range entangled phases

- Assume a symmetry G and excitation gap Δ
- $H_1 \sim H_2$ if H_1 and H_2 are connected without breaking symmetry G or closing gap Δ (with or without ancillas)



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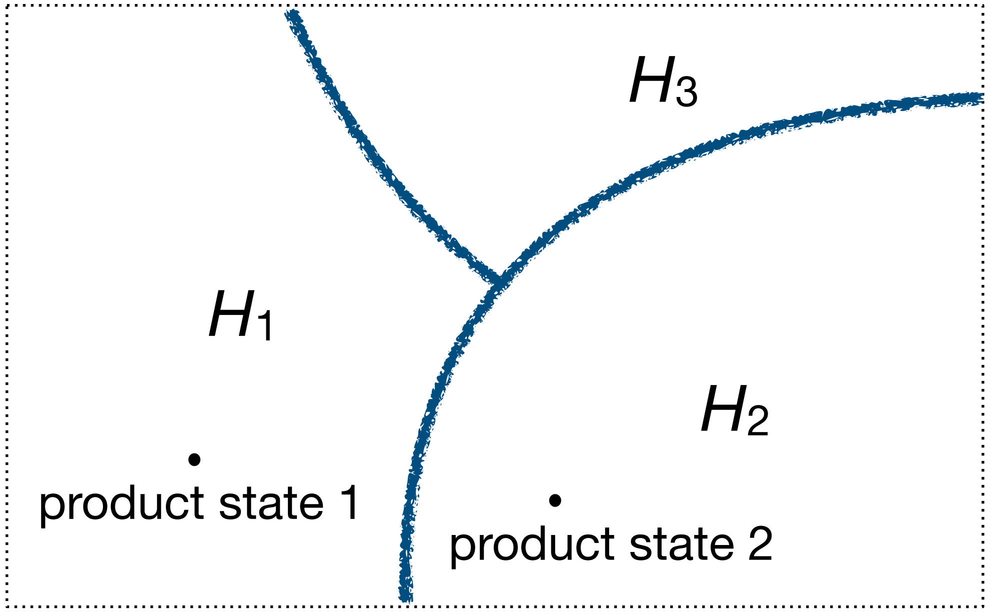
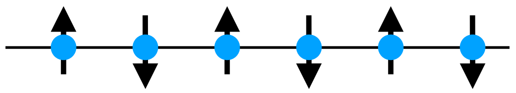


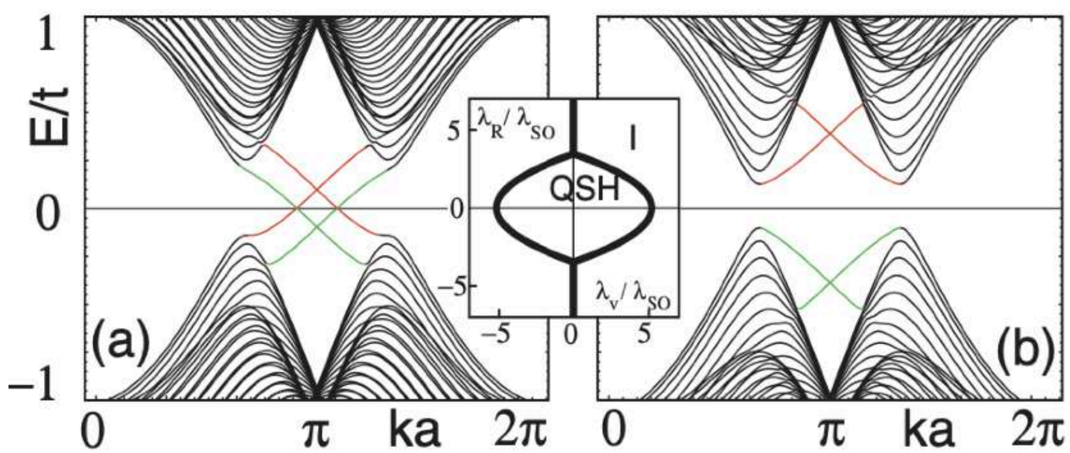
- *Trivial phases* are connected to a real-space **product state.**



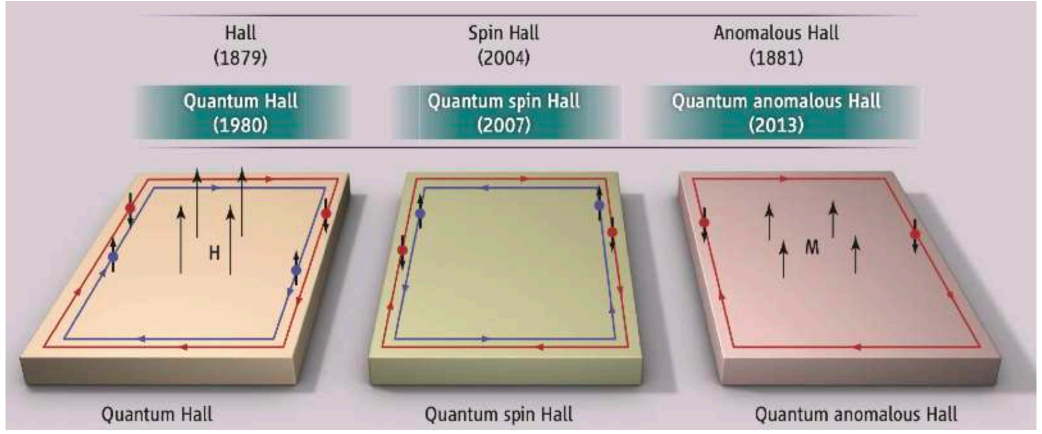
- *Topological phases* contain irremovable **quantum entanglement.**

Bulk-boundary correspondence of topological phases

- 2D topological insulator

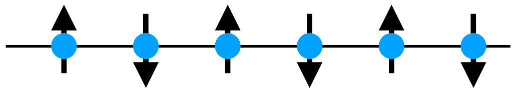


C. L. Kane and E. J. Mele, PRL (2005)



S. Oh, Science (2013)

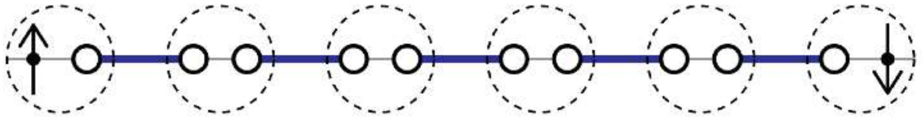
- Haldane phase

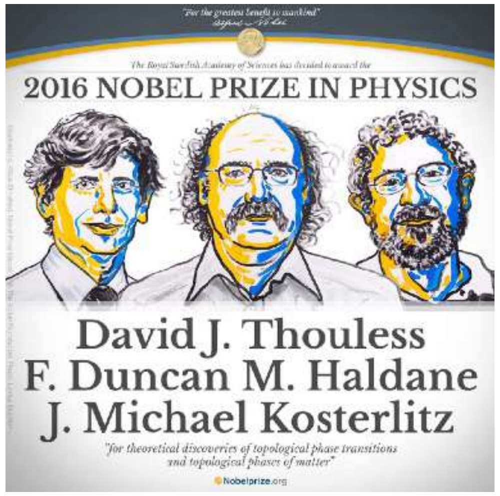


S = 1 Heisenberg model

$$\hat{H} = J \sum_n \hat{\boldsymbol{s}}_n \cdot \hat{\boldsymbol{s}}_{n+1}$$

S = 1/2 edge spin

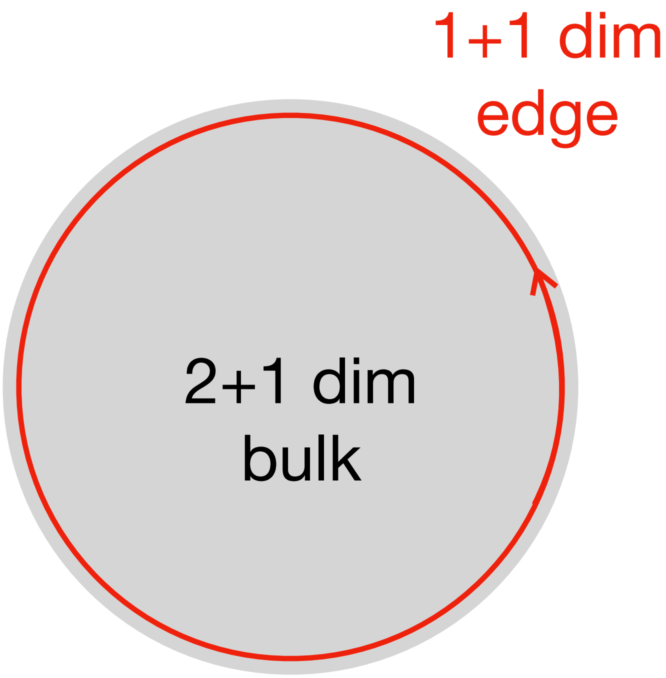




***Bulk* topology implies nontrivial *boundary*.**

Boundary states(=degrees of freedom) / surface topological order

Bulk-boundary correspondence
— anomaly inflow —

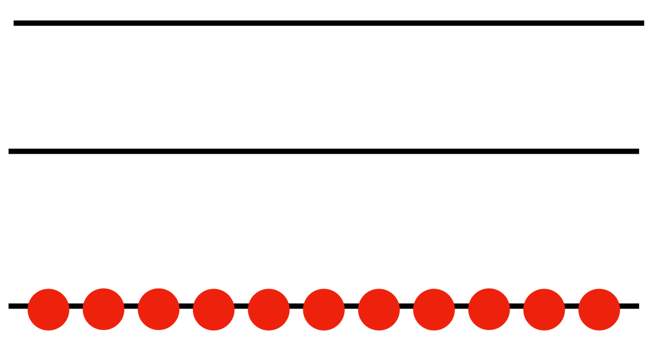


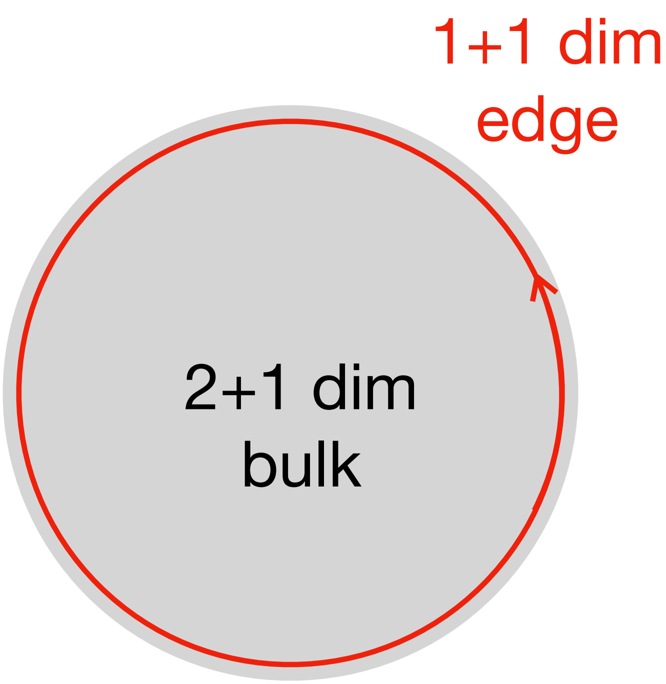
Bulk-boundary correspondence — anomaly inflow —

2+1 dim bulk:
Chern Simons theory

$$I_{\text{eff}} = \frac{k}{4\pi}\int_{M_3} \mathrm{d}^3x\epsilon^{ijk}A_i\partial_j A_k.$$

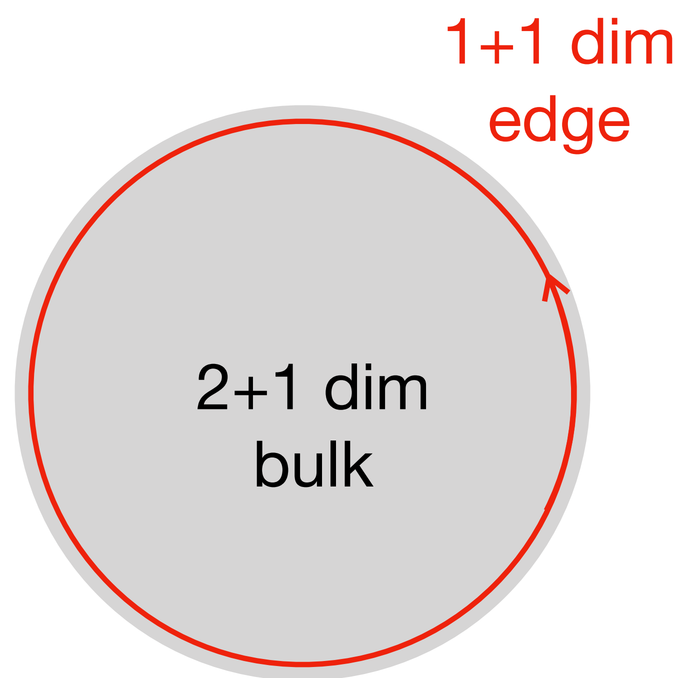
⋮





- Gauge invariant if no boundary
- Gauge dependent with boundary

Bulk-boundary correspondence — anomaly inflow —



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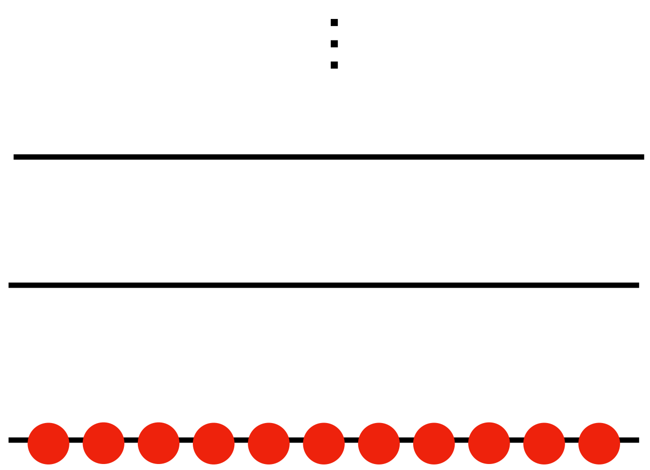
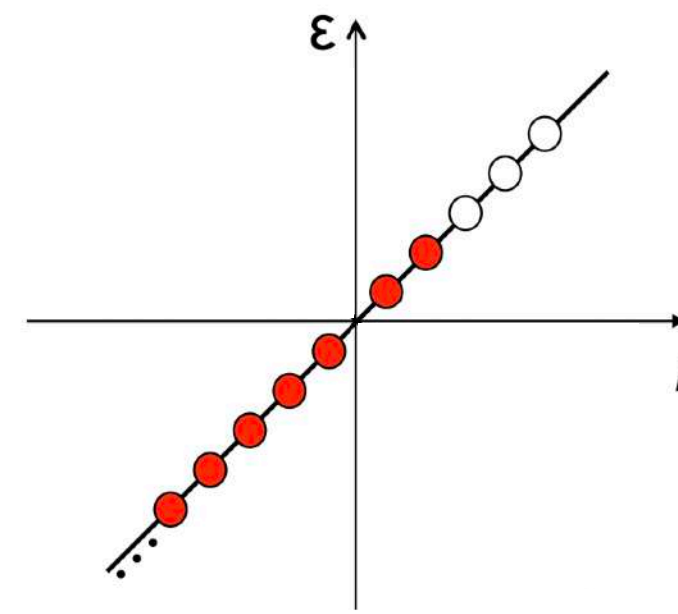


- Gauge invariant if no boundary
- Gauge dependent with boundary

1+1 dim edge
Chiral edge mode

$$H = v\int_{-\infty}^{\infty} \mathrm{d}x\ \psi^* \left(-\mathrm{i}\frac{\partial}{\partial x}\right)\psi .$$



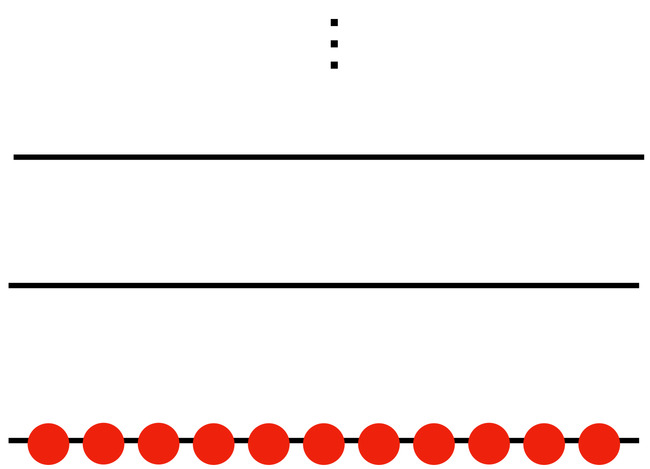
Chiral anomaly

$$\partial_\mu j^\mu = \mathrm{sign}(v)\,\frac{e^2 c}{4\pi\hbar}\epsilon^{\mu\nu}F_{\mu\nu}$$

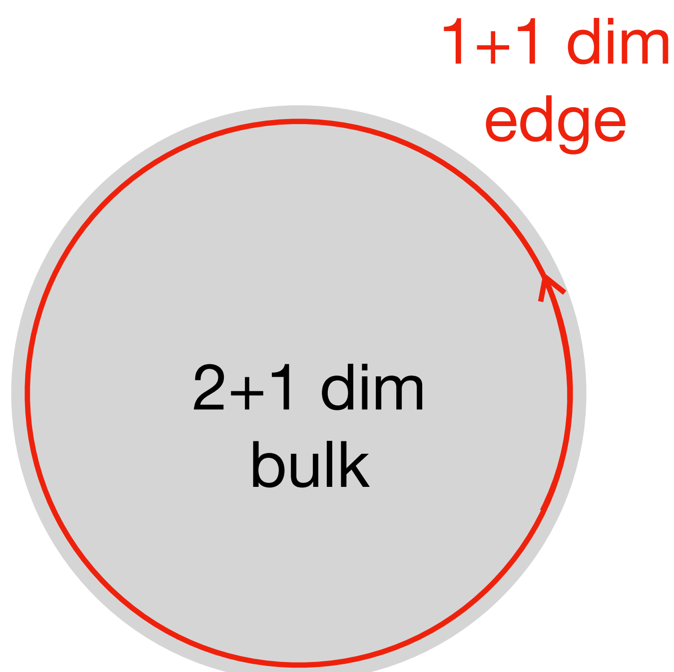
Bulk-boundary correspondence — anomaly inflow —

2+1 dim bulk:
Chern Simons theory

$$I_{\mathrm{eff}} = \frac{k}{4\pi}\int_{M_3} \mathrm{d}^3x\,\epsilon^{ijk}A_i\partial_j A_k.$$



- Gauge invariant if no boundary
- Gauge dependent with boundary

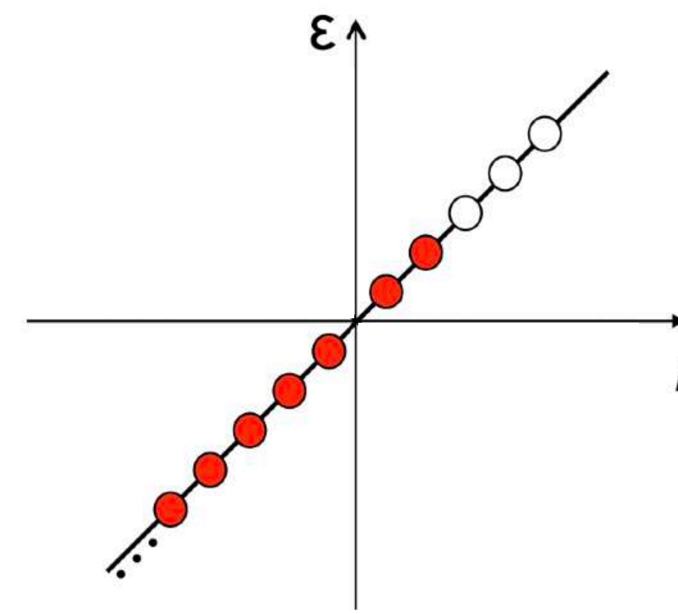


gauge dependence cancels between bulk and edge

robust against decoration / perturbation of surface

1+1 dim edge
Chiral edge mode

$$H = v\int_{-\infty}^{\infty}\mathrm{d}x\;\psi^*\left(-\mathrm{i}\frac{\partial}{\partial x}\right)\psi.$$



Chiral anomaly

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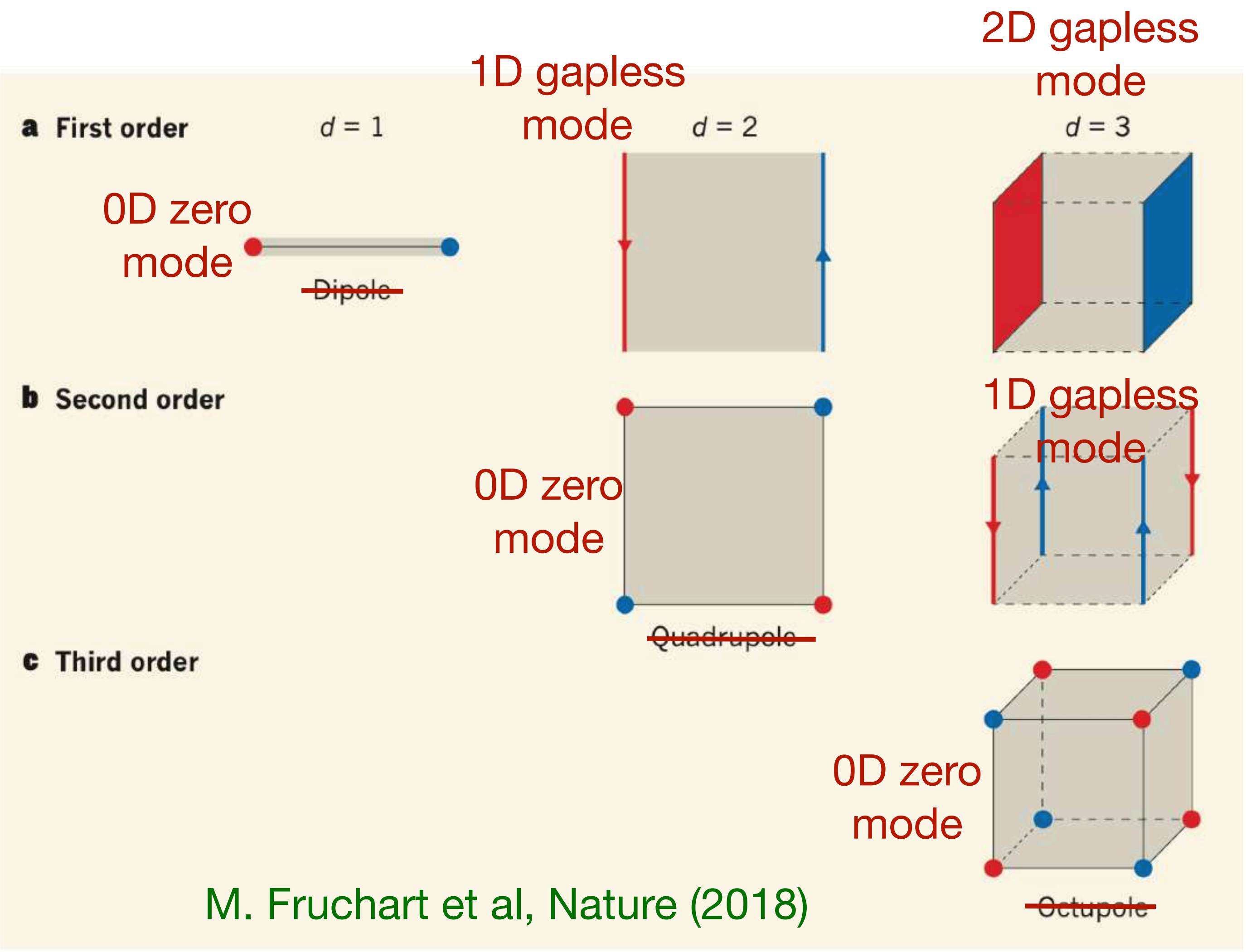
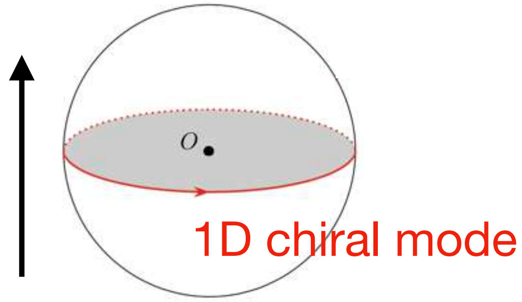
Bulk-boundary correspondence for higher-order topology

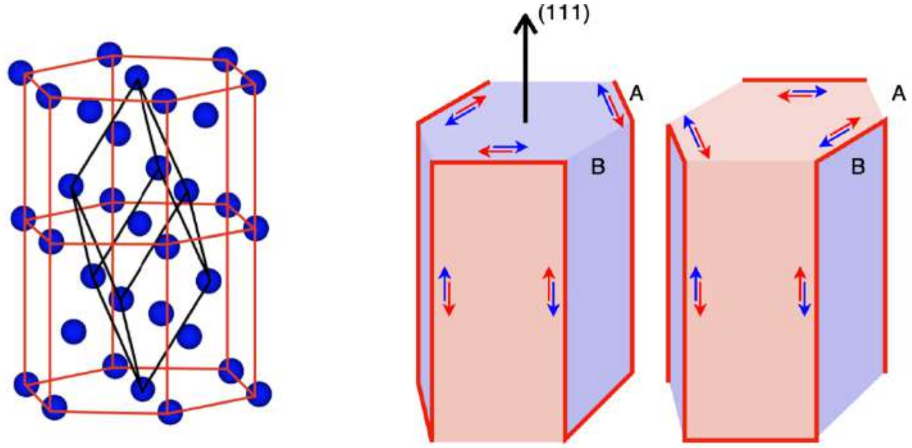


M. Fruchart et al, Nature (2018)

Inversion symmetric 3D topological insulator under magnetic field



Higher order topology in Bismuth

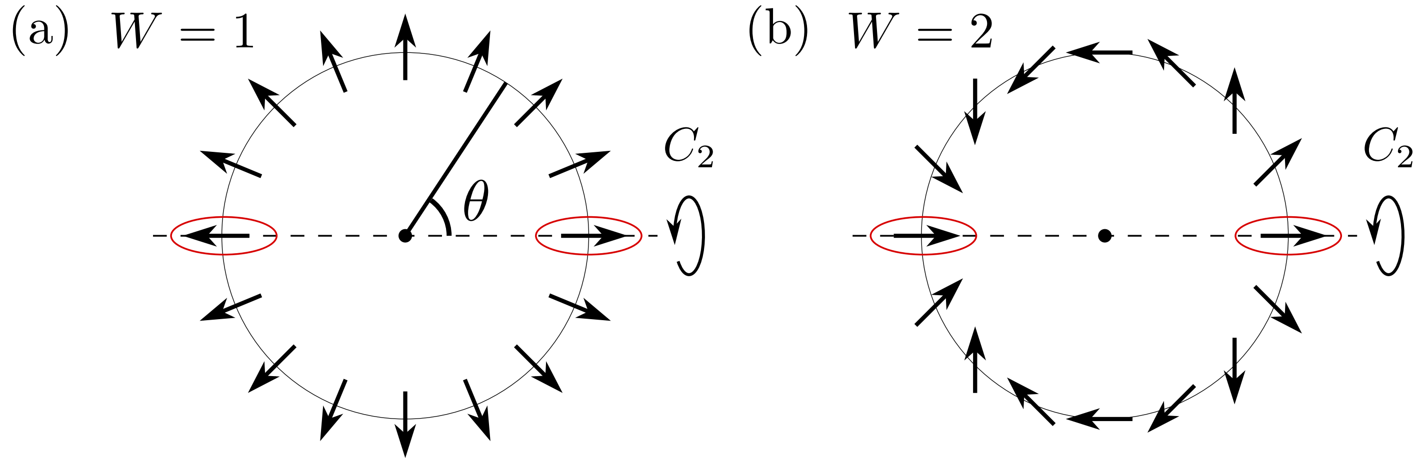


F. Schindler et al, Nature Physics (2018)
F. Schindler et al, Science Advances (2018)

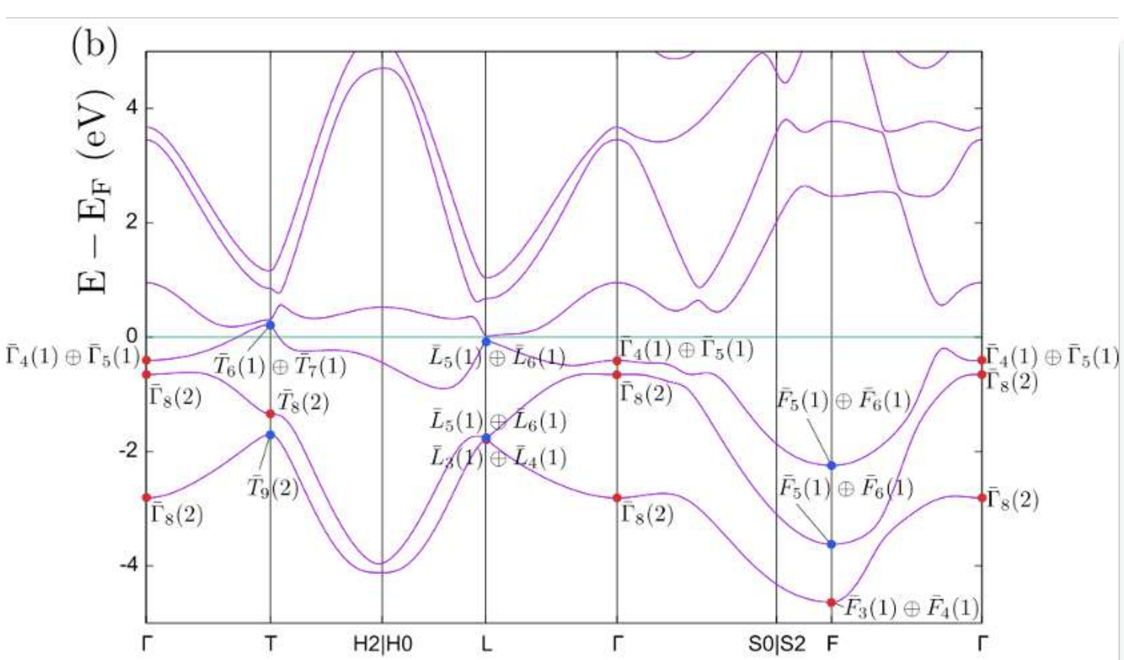
Boundary states can be localized to **corners** and **hinges** depending on the bulk topology.

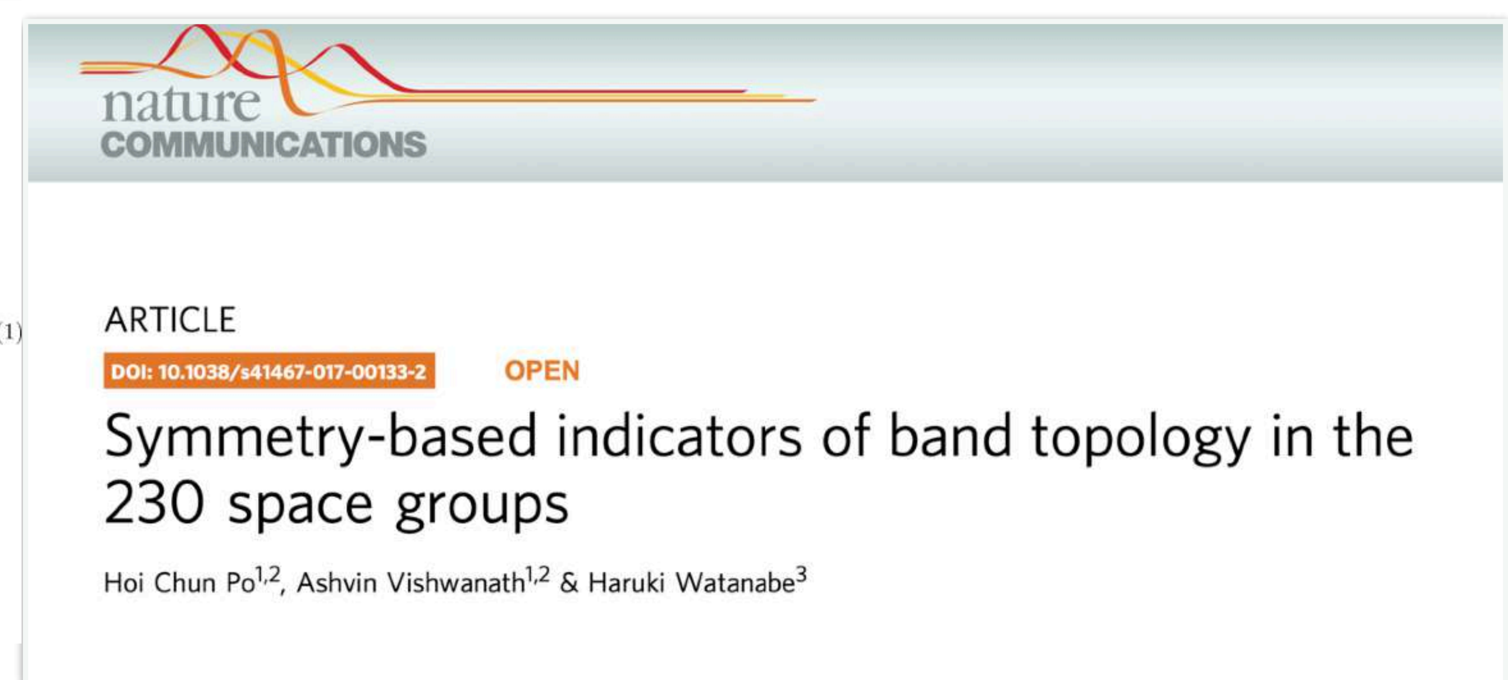
Symmetry indicators of band topology

- A handy diagnosis of topology



- Similar relation holds in the band structure of electrons in solids




nature COMMUNICATIONS

ARTICLE

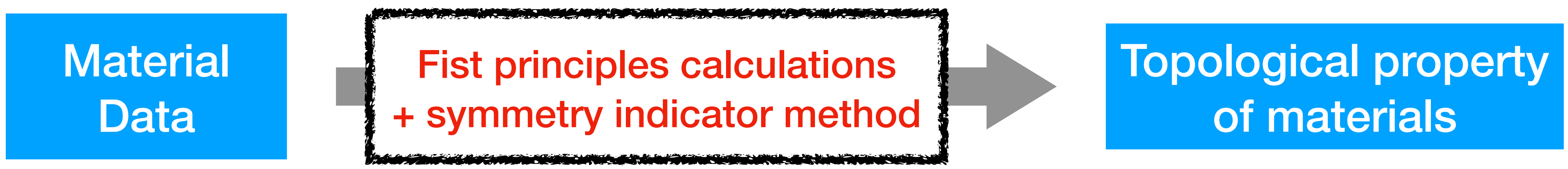
DOI: 10.1038/s41467-017-00133-2 OPEN

Symmetry-based indicators of band topology in the 230 space groups

Hoi Chun Po[1,2], Ashvin Vishwanath[1,2] & Haruki Watanabe[3]

A paradigm shift in material search

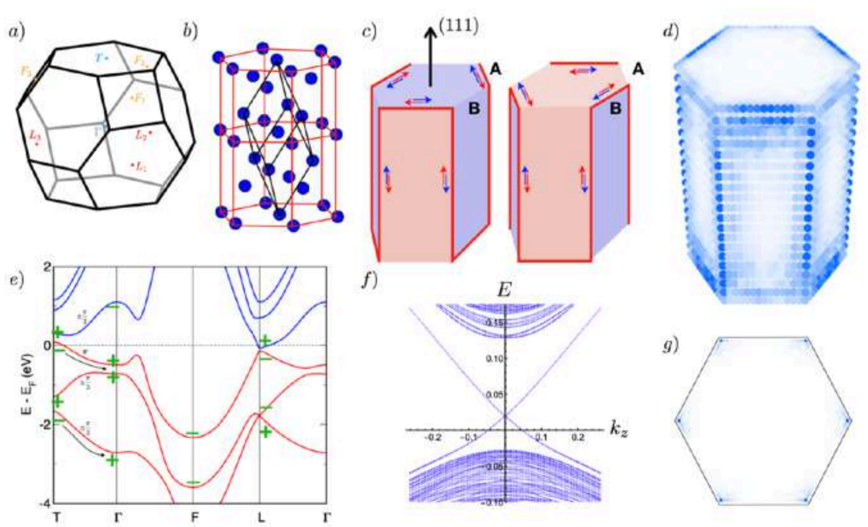
- Investigation of topological properties for *all* materials listed on database



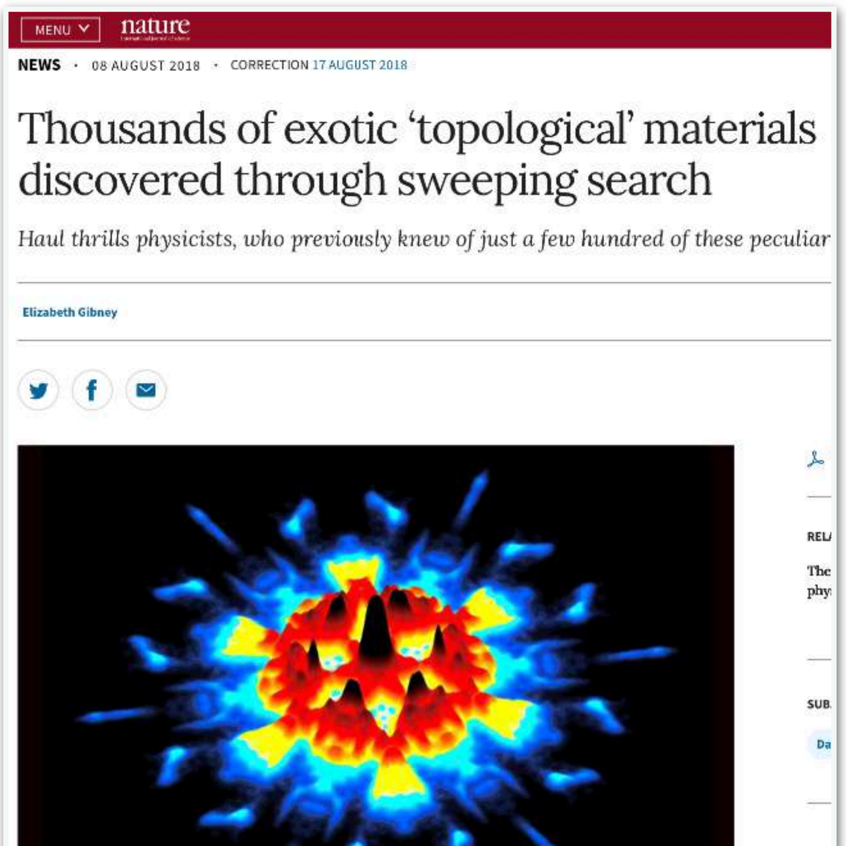
A paradigm shift in material search

- Investigation of topological properties for *all* materials listed on database

Material Data → Fist principles calculations + symmetry indicator method → Topological property of materials



Higher-order topology in Bismuth
Schindler *et al*, Nat. Phys. (2018)

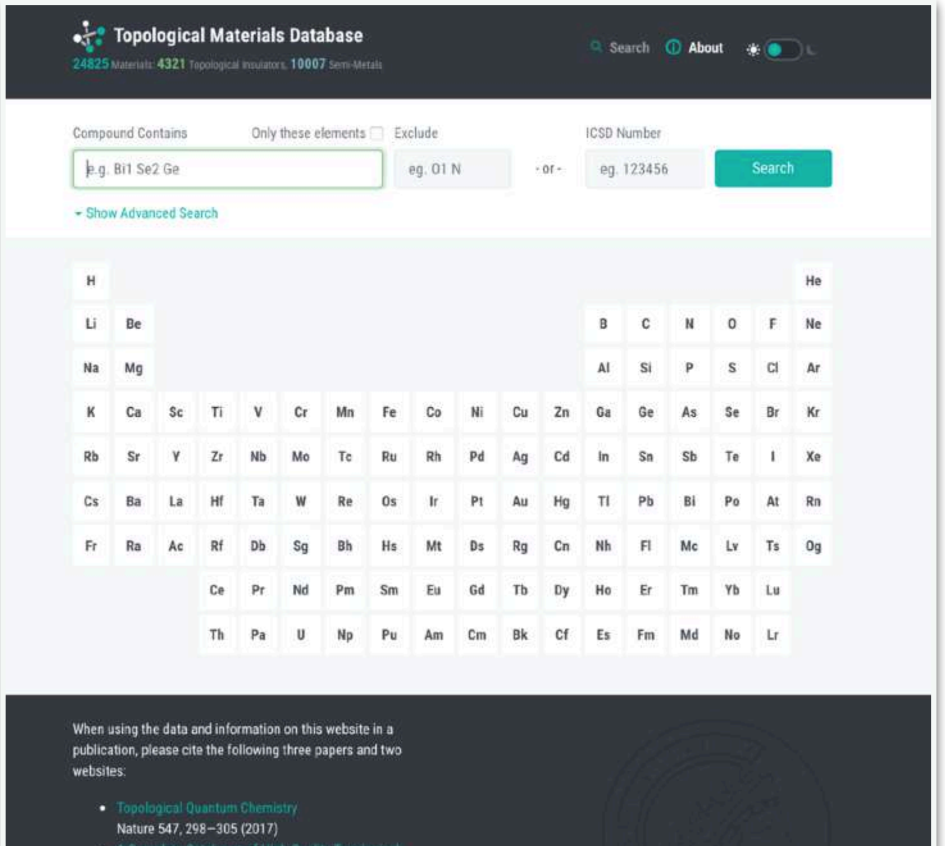

MENU nature

NEWS · 08 AUGUST 2018 · CORRECTION 17 AUGUST 2018

Thousands of exotic 'topological' materials discovered through sweeping search

Haul thrills physicists, who previously knew of just a few hundred of these peculiar

Elizabeth Gibney


Topological Materials Database

24825 Materials: 4321 Topological Insulators, 10007 Semi-Metals

Search About

Compound Contains | Only these elements | Exclude | ICSD Number

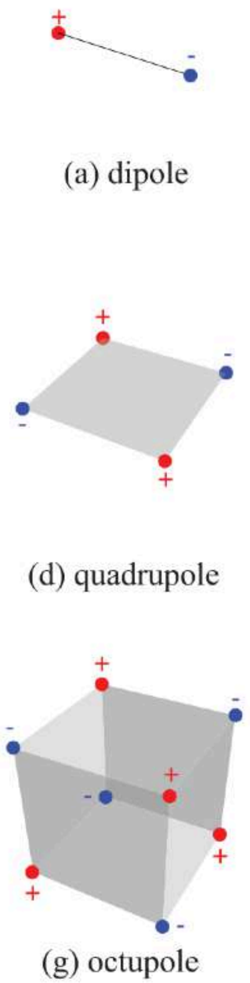
e.g. Bi1 Se2 Ge | eg. O1 N | - or - | eg. 123456 | Search

Show Advanced Search

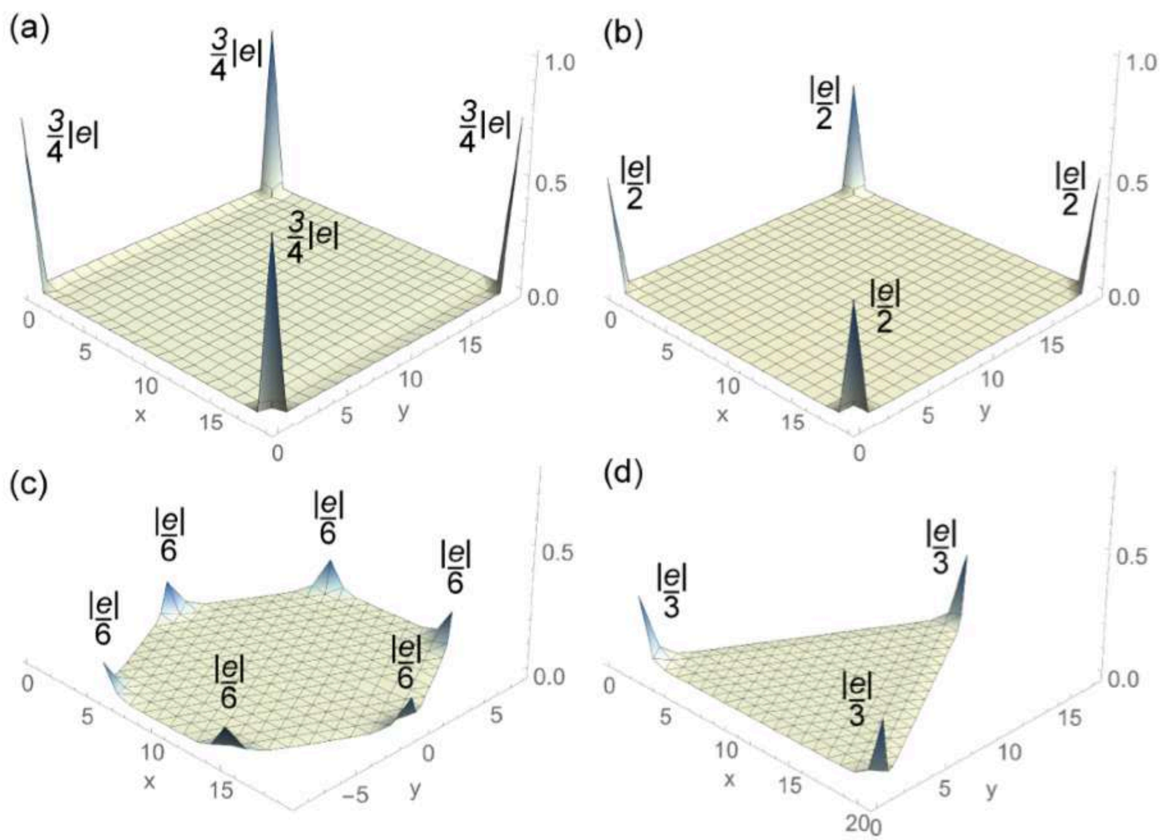
When using the data and information on this website in a publication, please cite the following three papers and two websites:

- Topological Quantum Chemistry
Nature 547, 298–305 (2017)

Bulk-boundary correspondence of *trivial* insulators



W. A. Benalcazar, B. A. Bernevig, T. L. Hughes, Science (2017) / PRB (2017)



Fractionally quantized
→ something topological

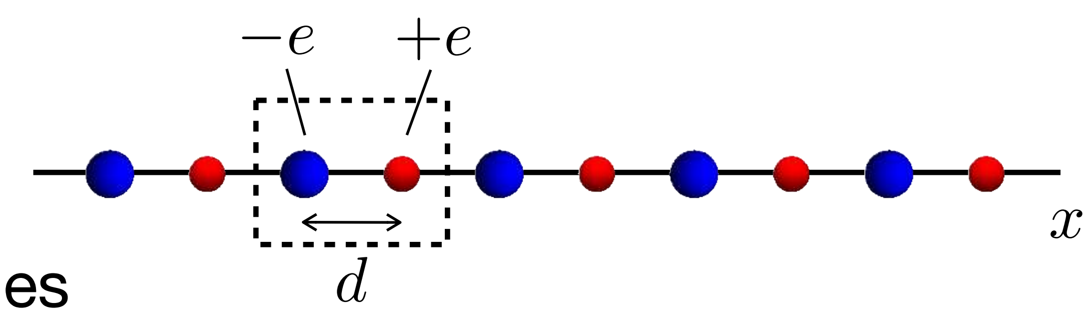
W. A. Benalcazar, T. Li, T. L. Hughes, PRB (2019)

Bulk **multipole moment implies** ***boundary*** **charges.**

Charges are “frozen” i.e., *not* degrees of freedom

Polarization and Edge charge

- Assume **U(1) symmetry** and **translation symmetry**



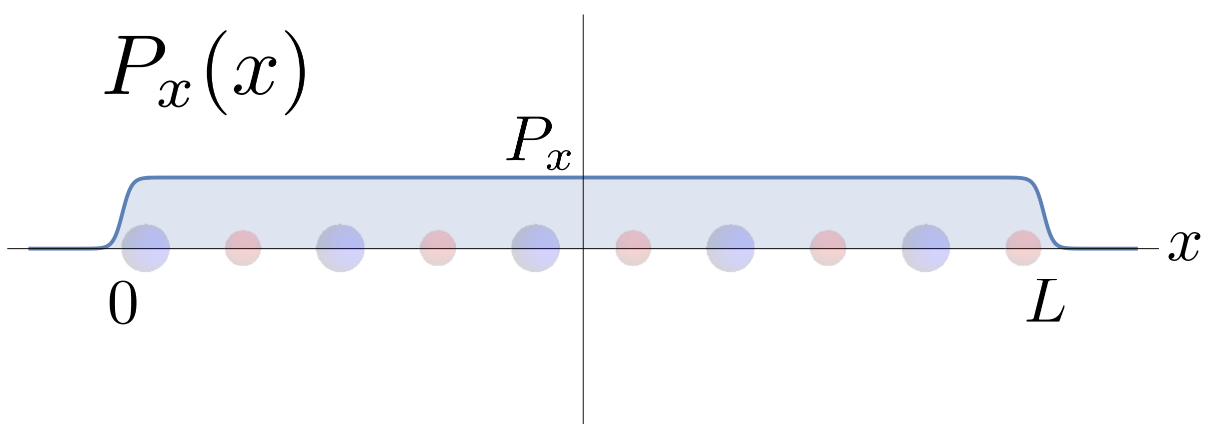
- For classical point charges

$$P_x^{(\text{classical})} = \frac{1}{a} \sum_{i \in \text{unit cell}} Q_i x_i = \frac{(-e)(x_0) + (+e)(x_0 + d)}{a} = e\frac{d}{a}$$

$$Q_{\text{edge}} \equiv -\int_{\text{edge}} dx\, \partial_x P(x) = P_x$$

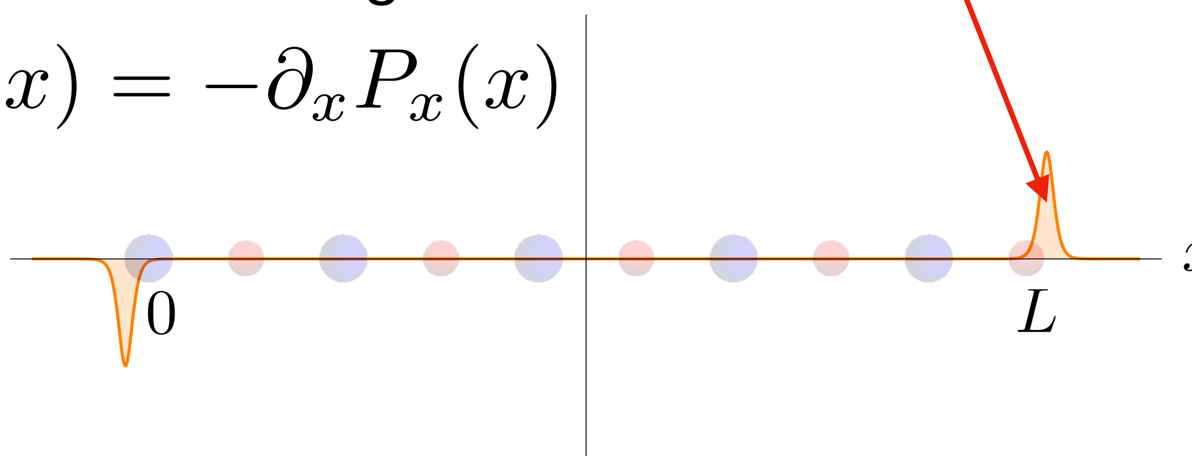
Polarization

$P_x(x)$



Polarization charge

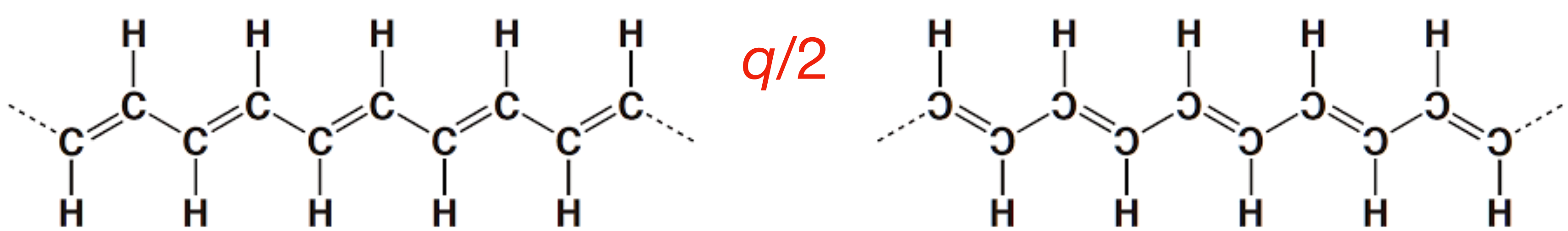
$\rho(x) = -\partial_x P_x(x)$

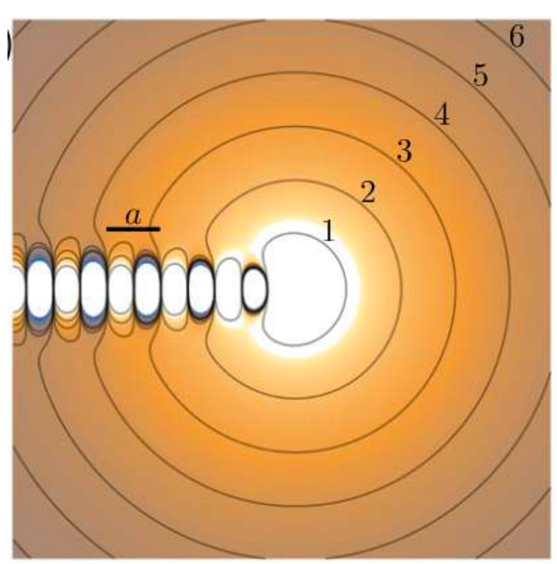


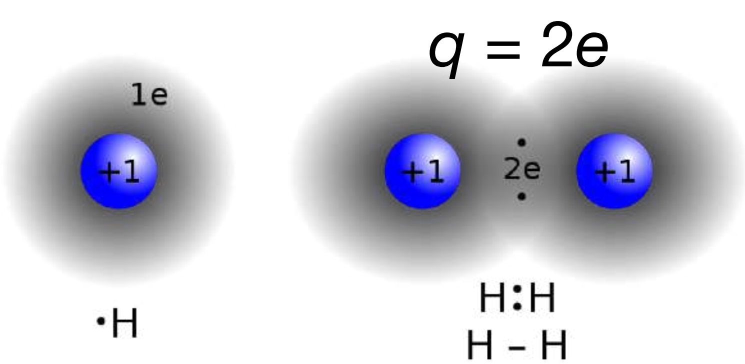
Edge **charge is given by** ***bulk*** **polarization!**

Solitons in polyacetylene

- R. Jackiw and C. Rebbi, “Solitons with fermion number 1/2,” PRD (1976).
- W. P. Su, J. R. Schrieffer, and A. J. Heeger, “Solitons in polyacetylene,” PRL (1979).
- A. J. Heeger, S. Kivelson, J. R. Schrieffer, and W. P. Su, “Solitons in conducting polymers,” RMP (1988).



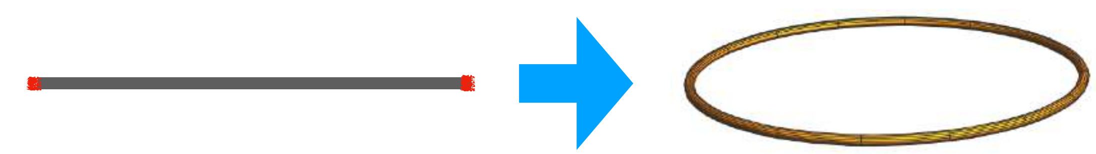




from: wikipedia

Formula of bulk polarization "Modern theory"

- Periodic Boundary Condition (PBC): $\hat{c}^{\dagger}_{x+L} = \hat{c}^{\dagger}_{x}$



$x \sim x + L$

- Conserved U(1) charge and polarization operator

$$\hat{Q} \equiv \int_0^L dx\, \hat{\rho}(x) \qquad \hat{P}_x \equiv \frac{1}{L}\int_0^L dx\, x\hat{\rho}(x)$$

$\hat{P}_x$ is inconsistent with PBC.
$\langle \hat{P}_x \rangle$ does not work in general!

- Berry phase formula

$$P_x = \langle \hat{P}_x \rangle + \frac{e}{2\pi}\gamma$$

Band insulators

R. D. King-Smith, D. VanderbiltPRB (1993)

$$\gamma = -\sum_{n\in\mathrm{occ}} \int_0^{\frac{2\pi}{a}} dk\, u^*_{nk} i\partial_k u_{nk}$$

$u_{n\,k+\frac{2\pi}{a}} = u_{nk}$

$i\partial_k \sim x$

Interacting systems

G. Ortiz, R. M. Martin, PRB (1994)
HW, M. Oshikawa, PRX (2017)

$$\gamma = -\int_0^{2\pi} d\phi\, i\langle\phi|\partial_\phi|\phi\rangle$$

Twisted Boundary Condition

$\hat{c}^{\dagger}_{x+L} = e^{-i\phi}\hat{c}^{\dagger}_{x} \qquad |\phi + 2\pi\rangle = |\phi\rangle$

- Resta's formula

$$P_x = \frac{e}{2\pi}\mathrm{Im}\log\left\langle e^{i2\pi\hat{P}_x/e}\right\rangle$$

R. Resta, PRL (1998)

We know how to compute the bulk P_x even for interacting systems!

Formula of bulk higher-order multipoles?

- Difficulties in generalizing the Berry phase formula

$$\sum_{n\in\mathrm{occ}}\int_{\mathrm{BZ}}\frac{dk_x}{2\pi}u^*_{nk_x}i\partial_{k_x}u_{nk_x}\to\sum_{n\in\mathrm{occ}}\int_{\mathrm{BZ}}\frac{d^2k}{(2\pi)^2}u^*_{n\boldsymbol{k}}i\partial_{k_x}i\partial_{k_y}u_{n\boldsymbol{k}}$$

→gauge dependent

$i\partial_{k_x}i\partial_{k_y}\sim xy$ $\quad u_{n\boldsymbol{k}}\to e^{i\theta_{\boldsymbol{k}}}u_{n\boldsymbol{k}}$

- Attemps in generalizing Resta's formula

$$\left\langle e^{2\pi i\int_0^{L_x}dx\,\frac{x}{L_x}\frac{\hat{\rho}(x)}{e}}\right\rangle\to\left\langle e^{2\pi i\int_0^{L_x}dx\int_0^{L_y}dy\,\frac{xy}{L_xL_y}\frac{\hat{\rho}(x,y)}{e}}\right\rangle$$

B. Kang, K. Shiozaki, G. Y. Cho, PRB (2019)
W. A. Wheeler, L. K. Wagner, T. L. Hughes, PRB (2019)
S. Ono, L. Trifunovic, HW, PRB (2019)

- Nested Wilson loop approach for band insulators (gives only the edge polarization.)

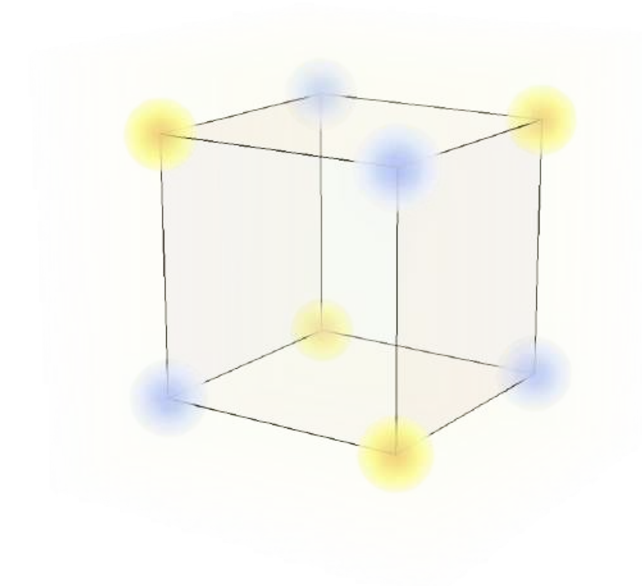
W. A. Benalcazar, B. A. Bernevig, T. L. Hughes, Science (2017) / PRB (2017)

- More direct generalization of the “modern theory”?

HW, S. Ono, PRB (2020)
L. Trifunovic, PRR (2020)
S. H. Kooi, G. van Miert, C. Ortix, npj QM (2021)
S. Ren, I. Souza, D. Vanderbilt, PRB (2021)

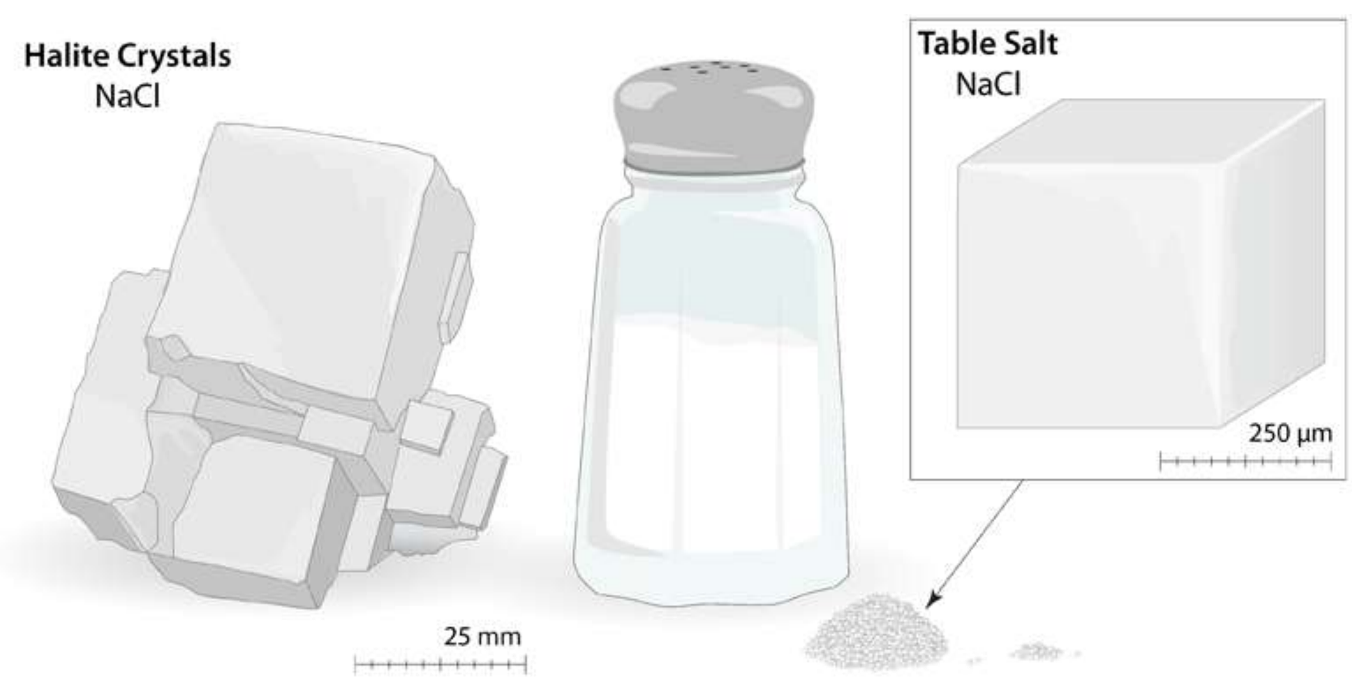
Our goal

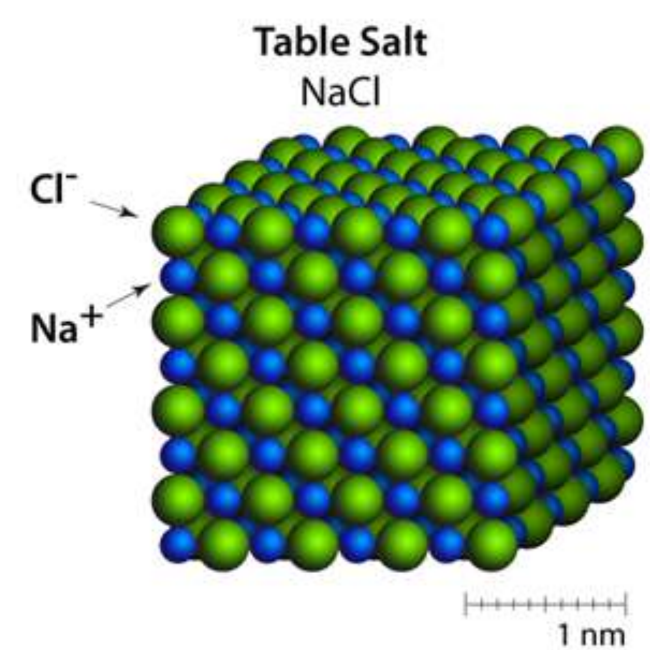
1. Give a general formulation of the bulk multipole moments
   → Characterization of trivial phases of matter



2. Clarify the relation to corner / hinges charges

3. Propose materials / experiments



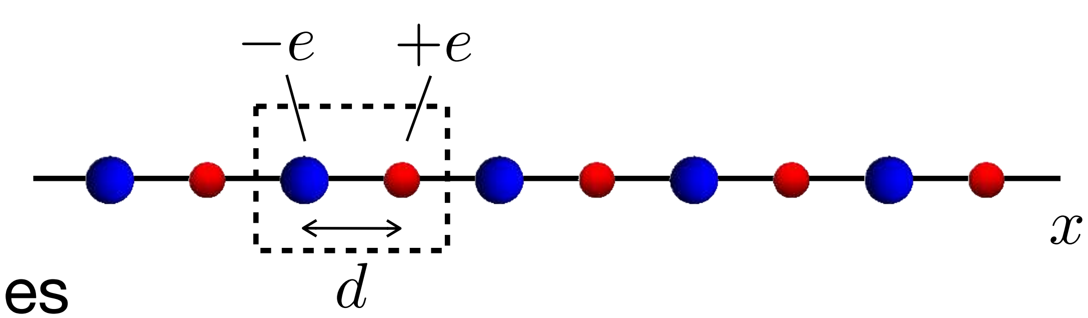


Images from http://www.atomsinmotion.com/book/chapter4/salts

Polarization in 1D systems

Polarization and Edge charge

- Assume **U(1) symmetry** and **translation symmetry**

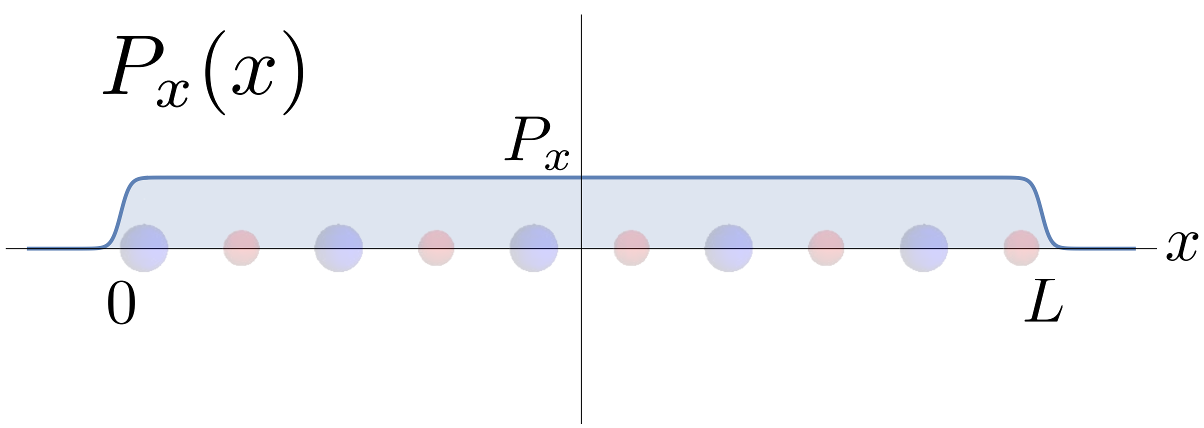


- For classical point charges

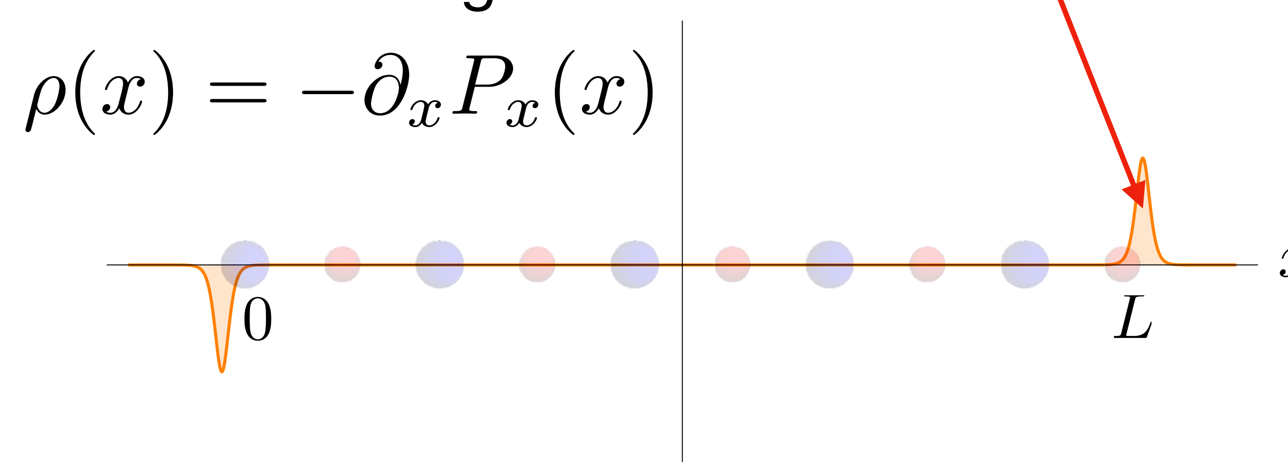
$$P_x^{(\text{classical})} = \frac{1}{a} \sum_{i \in \text{unit cell}} Q_i x_i = \frac{(-e)(x_0) + (+e)(x_0 + d)}{a} = e\frac{d}{a}$$

$$Q_{\text{edge}} \equiv -\int_{\text{edge}} dx\, \partial_x P(x) = P_x$$

Polarization

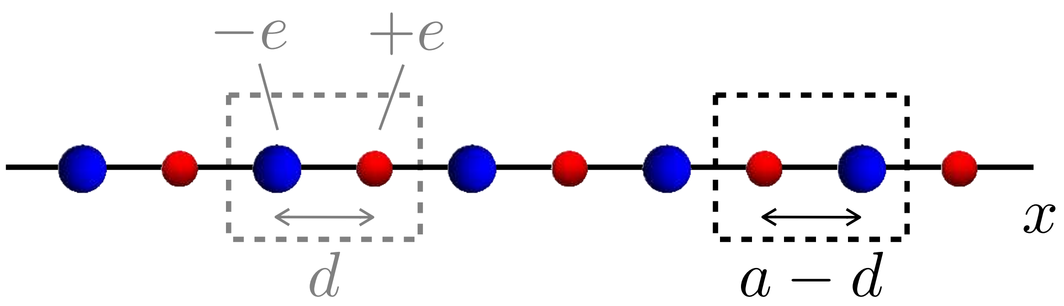


Polarization charge



***Edge* charge is given by *bulk* polarization!**

Ambiguity of bulk polarization

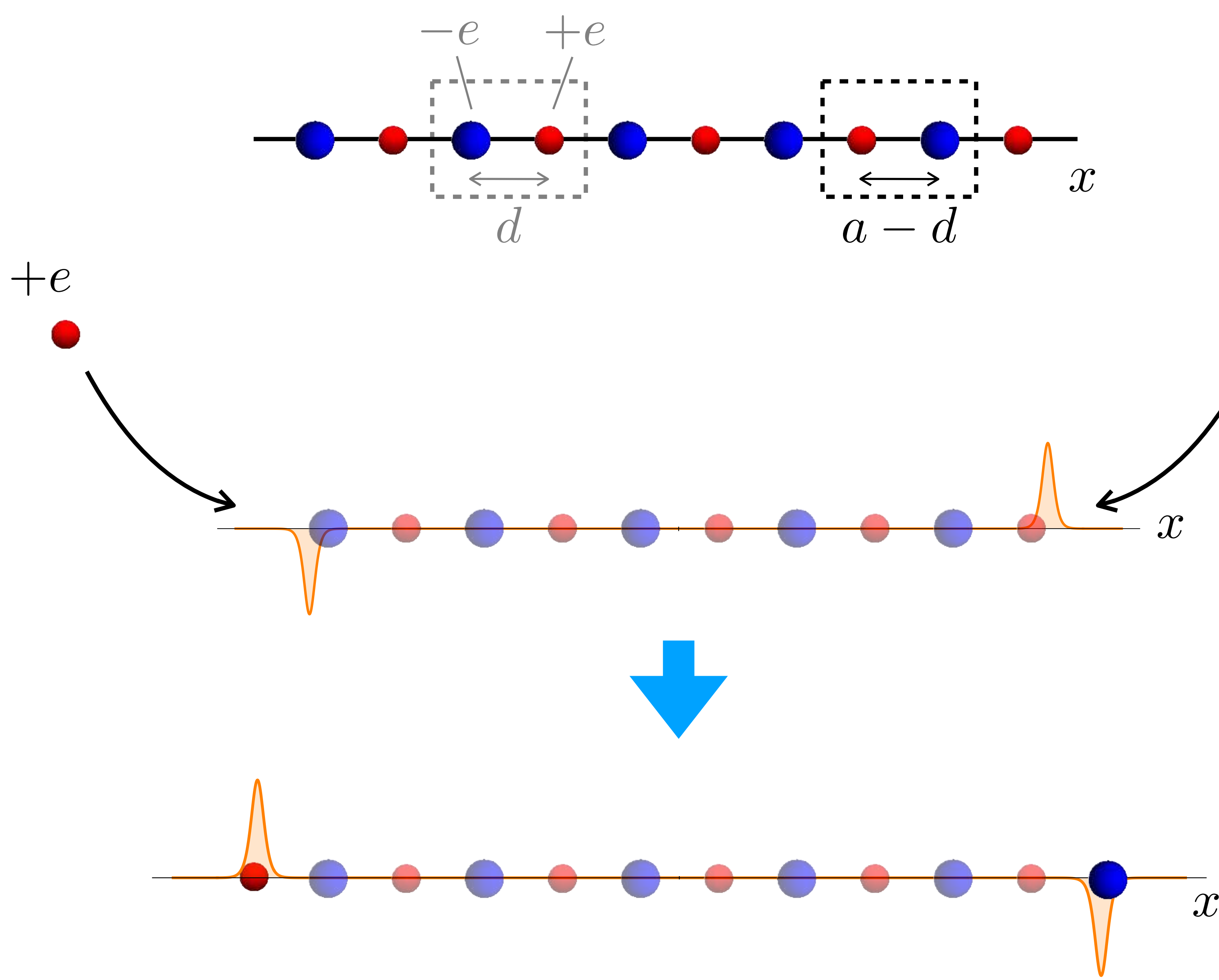


$$P_x^{(\text{classical})} = \frac{1}{a} \sum_{i \in \text{unit cell}} Q_i x_i = \frac{(-e)(x_0) + (+e)(x_0 + d)}{a} = e\frac{d}{a}$$

$$P_x^{(\text{classical})} = \frac{1}{a} \sum_{i \in \text{unit cell}} Q_i x_i = \frac{(-e)(x_0) + (+e)(x_0 + d - a)}{a} = e\frac{d}{a} - e$$

Bulk polarization has an integer ambiguity.
(Choice of unit cell)

Ambiguity of edge charge



Edge charge also has an integer ambiguity.
(Choice of edge termination & decoration)

Quantization under symmetry

- Assume **inversion symmetry (*x*→–*x*)** in addition to **U(1)** and **translation**.

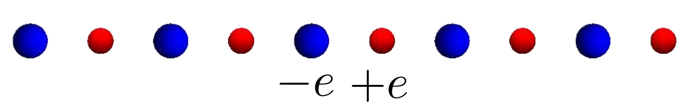
- Inversion symmetry flips the sign of polarization → quantization to 0 or e/2.

$$-P_x = P_x \mod e \quad \Rightarrow \quad P_x = 0 \text{ or } \frac{1}{2}e \mod e$$

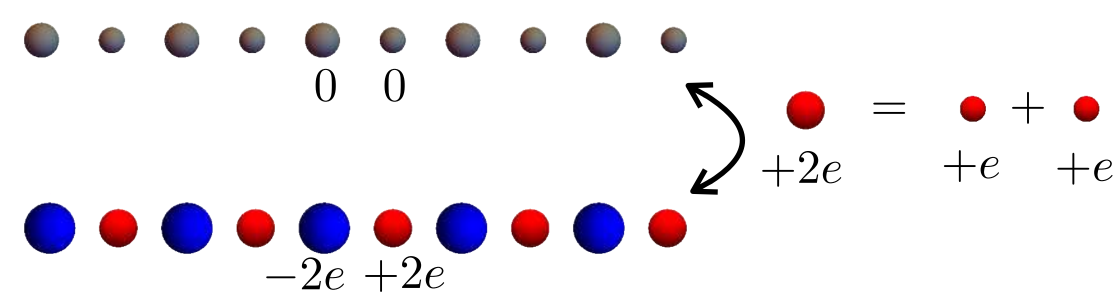
- There are at least two phases → trivial phases are not unique!

Y. Fuji, F. Pollmann, M. Oshikawa, PRL (2015)
H. C. Po, A. Vishwanath, HW, Nature Comm (2017)
+ many other works in the context of TCI

$$P_x = \frac{1}{2} \mod e$$



$$P_x = 0 \mod e$$

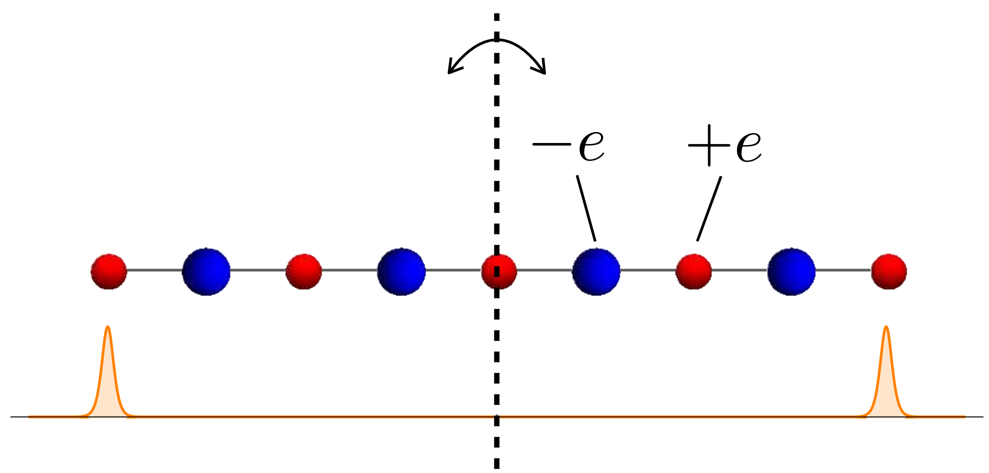


The U(1) charge *Q* mod 2*e* at the inversion center is a topological invariant.

“Filling anomaly”

- Sometimes **charge neutrality** and **point-group symmetry** cannot be simultaneously respected.

W. A. Benalcazar, T. Li, T. L. Hughes, PRB (2019)



$$Q_{\text{tot}} = +e$$

$$Q_{\text{edge}} = \frac{1}{2} Q_{\text{tot}} \mod e$$

Note:

1. This formula assumes charges are localized to edges.
2. Termination has to be designed carefully.

"Filling anomaly"

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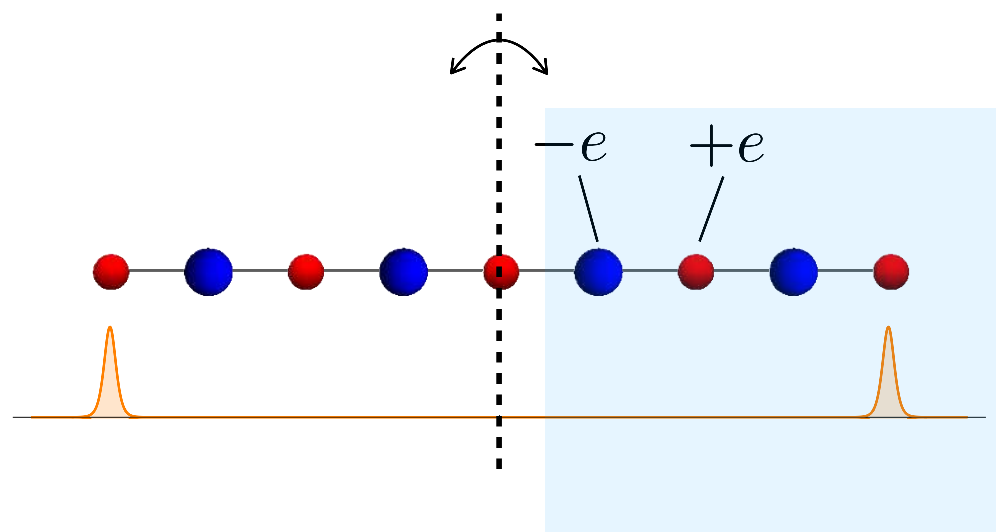
W. A. Benalcazar, T. Li, T. L. Hughes, PRB (2019)



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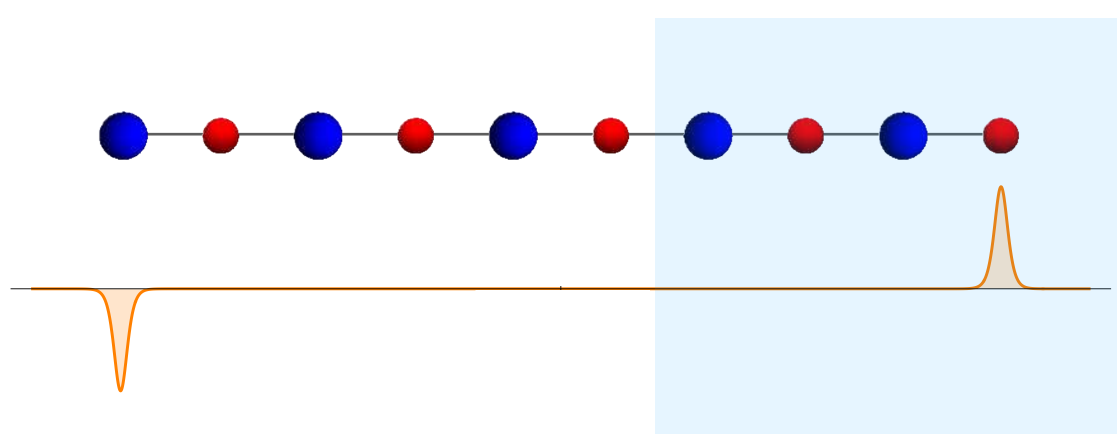


$$Q_{\text{tot}} = 0$$

Corner charge is a local property.
Not affected by the other edge

Definition of the edge charge

- Conserved charge of the U(1) symmetry:

$$\hat{Q} = \int dx \hat{\rho}(x)$$

- Microscopic charge density:

$$\rho^{(\mathrm{micro})}(x) = \langle \hat{\rho}(x) \rangle$$

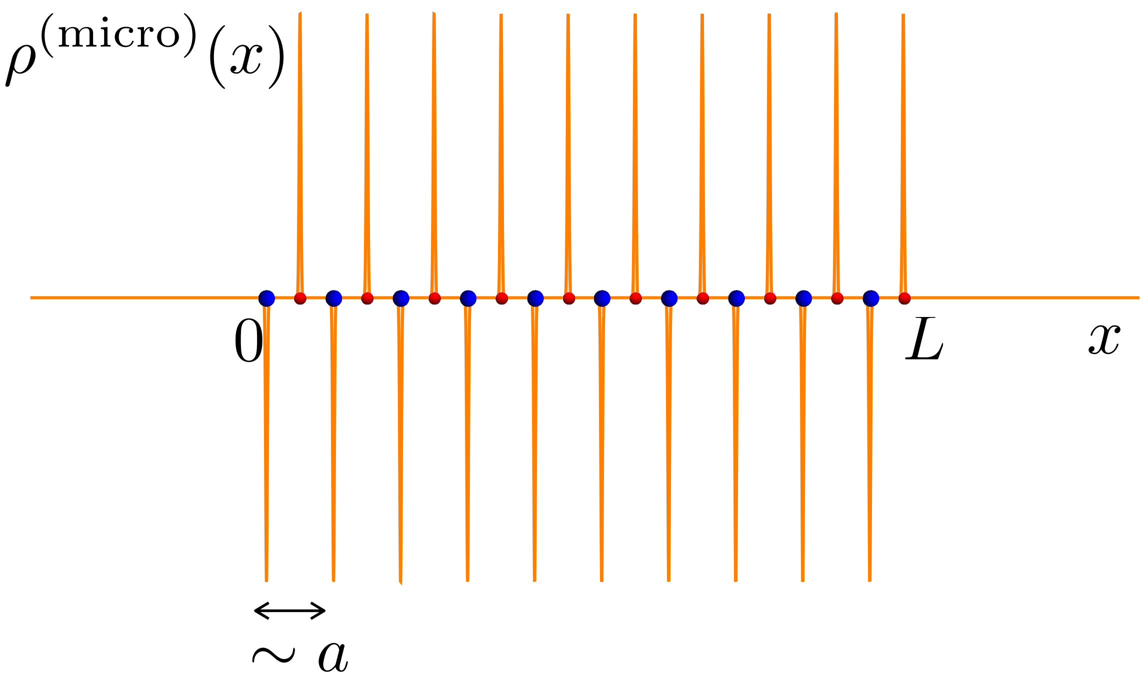
- Coarse-grained charge density:

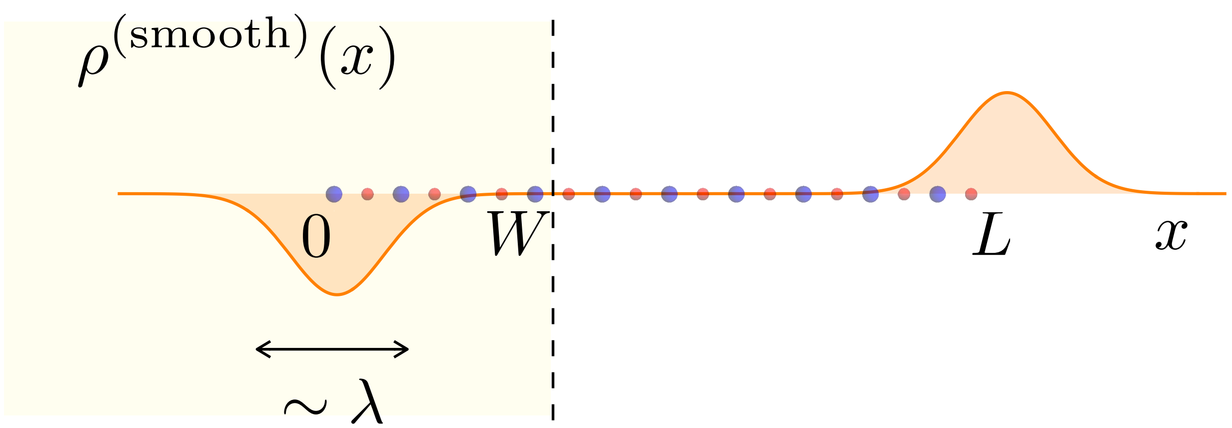
$$\rho^{(\mathrm{smooth})}(x) \equiv \int_{-\infty}^{\infty} dx' \, g(x-x') \rho^{(\mathrm{micro})}(x')$$

$$g(x) = \frac{1}{\sqrt{2\pi\lambda^2}} e^{-\frac{1}{2\lambda^2}x^2}$$

- Definition of edge charge:

$$Q_{\mathrm{edge}} \equiv \int_{-\infty}^{W} dx \, \rho^{(\mathrm{smooth})}(x)$$



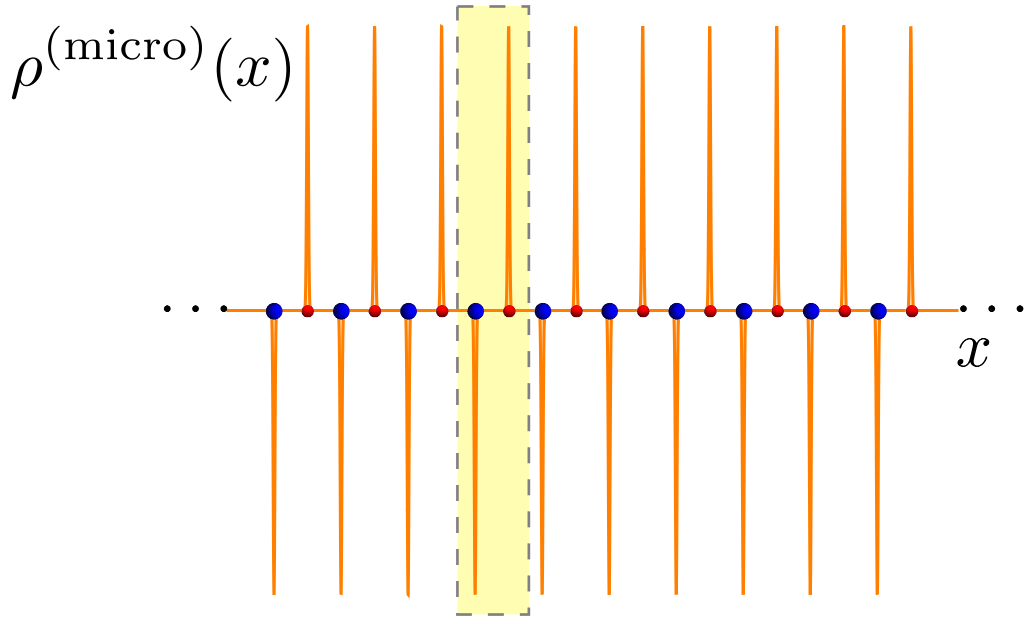


$$a \ll \lambda \ll W \ll L$$

(Definition of the bulk polarization)

- Translation invariance
  → a repetition unit of charge density

$$\rho^{(\mathrm{micro})}(x) = \sum_{n=-\infty}^{+\infty} \rho_0(x - na)$$



$\rho_0(x)$ is not unique.

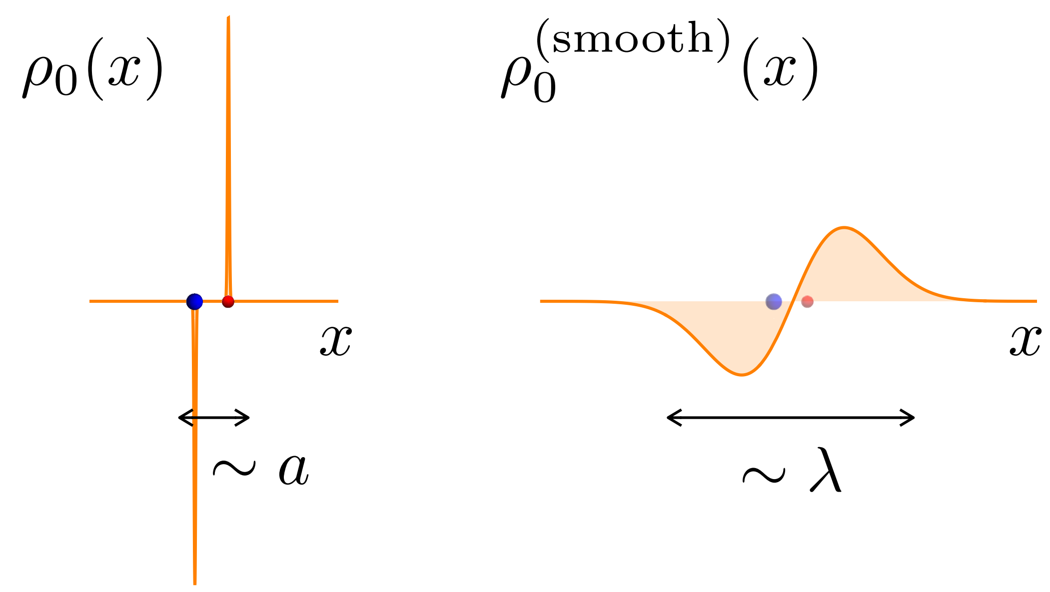
We require
$$\begin{cases} \rho_0(x) \to 0 \quad \text{when } |x| \gg a \\ \int_{-\infty}^{\infty} dx\, \rho_0(x) = 0 \end{cases}$$

- Definition of bulk polarization

$$P_x \equiv \frac{1}{a} \int_{-\infty}^{\infty} dx\, x \rho_0(x)$$

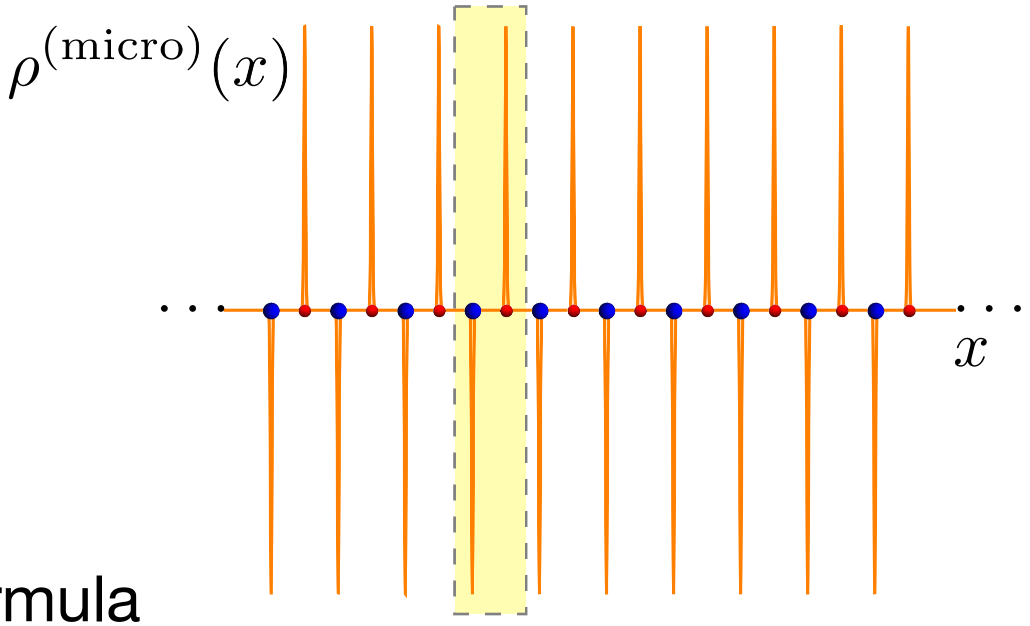
$$\left(= \frac{1}{a} \int_{-\infty}^{\infty} dx\, x \rho_0^{(\mathrm{smooth})}(x) \right)$$

$$\rho_0^{(\mathrm{smooth})}(x) \equiv \int_{-\infty}^{\infty} dx'\, g(x - x') \rho_0(x)$$



(Definition of the bulk polarization)

- For band insulators, $\rho_0(x)$ is given by Wannier function



$$\rho_0^{(\mathrm{el})}(x) = -\frac{ea}{L}\sum_{R}\sum_{n\in\mathrm{occ}} |w_{n,i}(R)|^2 \delta(x - R - x_i)$$

$$w_{n,i}(R) \sim \int_0^{\frac{2\pi}{a}} \frac{dk}{2\pi}\, u_{nk,i} e^{ikR}$$

- Our expression of P_x reduces to the Berry phase formula

$$P_x \equiv \frac{1}{a}\int_{-\infty}^{\infty} dx\, x\rho_0(x)$$

$$= \langle \hat{P}_x \rangle - e\sum_{n\in\mathrm{occ}} \int_0^{\frac{2\pi}{a}} \frac{dk}{2\pi} u_{nk}^* i\partial_k u_{nk}$$

(Proof of the bulk-edge correspondence)

Infinite system

$$\rho^{(\mathrm{micro})}(x) = \sum_{n=-\infty}^{+\infty} \rho_0(x - na)$$

Semi-infinite system

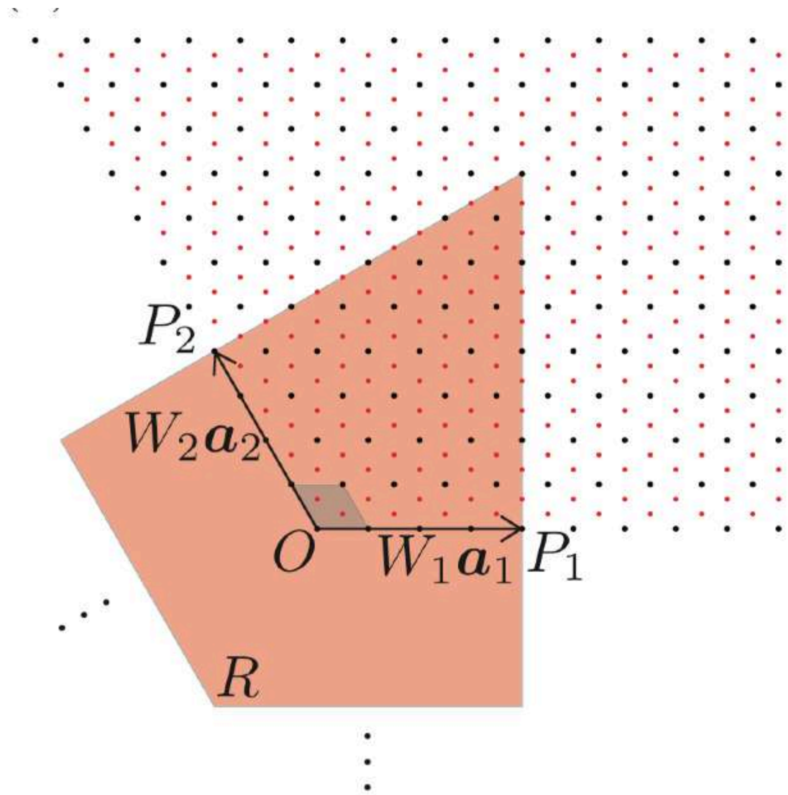
$$\rho^{(\mathrm{micro})}(x) = \sum_{n=0}^{+\infty} \rho_0(x - na)$$

$$\begin{aligned}
\rho^{(\mathrm{smooth})}(x) &\equiv \int_{-\infty}^{\infty} dx'\, g(x-x')\rho^{(\mathrm{micro})}(x) \\
&= \int_{-\infty}^{\infty} dx'\, g(x-x') \sum_{n=0}^{\infty} \rho_0(x-na) = \sum_{n=0}^{\infty} \rho_0^{(\mathrm{smooth})}(x-na) \\
&\underset{(\lambda \gg a)}{\simeq} \frac{1}{a}\int_{0}^{\infty} dx'\, \rho_0^{(\mathrm{smooth})}(x-x') = \frac{1}{a}\int_{-\infty}^{x} dx''\, \rho_0^{(\mathrm{smooth})}(x'')
\end{aligned}$$

$$\begin{aligned}
Q_{\mathrm{edge}} &\equiv \int_{-\infty}^{W} dx\, \rho^{(\mathrm{smooth})}(x) \\
&\simeq \frac{1}{a}\int_{-\infty}^{W} dx \int_{-\infty}^{x} dx'\, \rho_0^{(\mathrm{smooth})}(x') = \frac{1}{a}\int_{-\infty}^{W} dx' \int_{x'}^{W} dx\, \rho_0^{(\mathrm{smooth})}(x') \\
&= \frac{1}{a}\int_{-\infty}^{W} dx'\, (W-x')\rho_0^{(\mathrm{smooth})}(x') \simeq -\frac{1}{a}\int_{-\infty}^{\infty} dx'\, x'\rho_0^{(\mathrm{smooth})}(x') = -P_x
\end{aligned}$$

Higher order multipoles in higher D systems

2D: Quadrupole moment and corner charge



- Charge density

$$\rho^{(\mathrm{micro})}(\boldsymbol{r}) = \sum_{n_i \geq 0} \rho_0(\boldsymbol{r} - \textstyle\sum_{i=1}^{d} n_i \boldsymbol{a}_i).$$

- The total charge in the region *R*

$$Q_R = \int_R d^d r \rho^{(\mathrm{smooth})}(\boldsymbol{r}) = W_1 \sigma_2 + W_2 \sigma_1 + Q_{\mathrm{corner}}$$

- Surface charge density

$$\sigma_i = -\int_{\mathbb{R}^d} d^d r \rho_0(\boldsymbol{r}) P_i(\boldsymbol{r}) \qquad \boldsymbol{a}_i \cdot \boldsymbol{b}_j = \delta_{ij}$$

$$P_i(\boldsymbol{r}) \equiv \boldsymbol{b}_i \cdot \boldsymbol{r}$$

- Corner charge

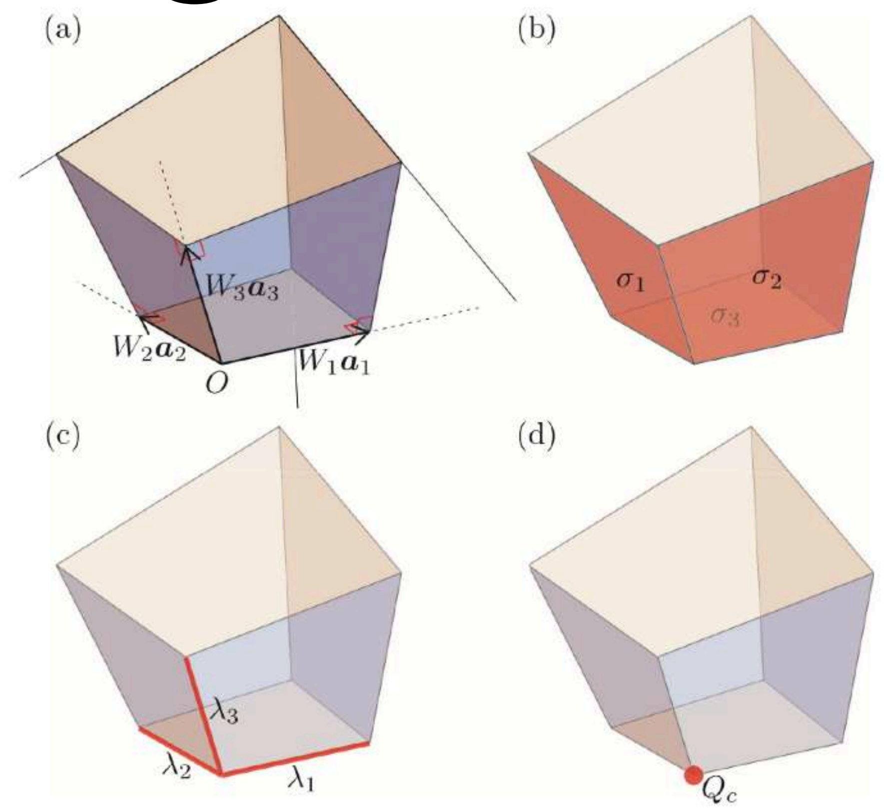
$$Q_{\mathrm{corner}} = \int_{\mathbb{R}^d} d^d r \rho_0(\boldsymbol{r}) Q_{12}(\boldsymbol{r})$$

$$Q_{12}(\boldsymbol{r}) \equiv (\boldsymbol{b}_1 \cdot \boldsymbol{r})(\boldsymbol{b}_2 \cdot \boldsymbol{r}) + \frac{\boldsymbol{a}_2 \cdot \boldsymbol{a}_1}{2a_2^2}(\boldsymbol{b}_1 \cdot \boldsymbol{r})^2 + \frac{\boldsymbol{a}_1 \cdot \boldsymbol{a}_2}{2a_1^2}(\boldsymbol{b}_2 \cdot \boldsymbol{r})^2$$

$$= \frac{1}{a_1 a_2}\left(\frac{x^2 - y^2}{2}\cos\theta + xy\sin\theta\right).$$

$$\boldsymbol{a}_1 = a_1(1, 0)$$
$$\boldsymbol{a}_2 = a_2(\cos\theta, \sin\theta)$$

3D: Octupole moment and corner/hinge charge



- Charge density

$$\rho^{(\mathrm{micro})}(\boldsymbol{r}) = \sum_{n_i \geq 0} \rho_0(\boldsymbol{r} - \textstyle\sum_{i=1}^{d} n_i \boldsymbol{a}_i).$$

- The total charge in the region *R*

$$Q_R = \int_R d^d r \rho^{(\mathrm{smooth})}(\boldsymbol{r}) = \sum_{i=1}^{3} S_i \sigma_i + \sum_{i=1}^{3} W_i \lambda_i + Q_{\mathrm{corner}}$$

- Hinge charge density

$$\lambda_3 = \int_{\mathbb{R}^d} d^d r \rho_0(\boldsymbol{r}) Q_{12}(\boldsymbol{r})$$

$$Q_{12}(\boldsymbol{r}) \equiv (\boldsymbol{b}_1 \cdot \boldsymbol{r})(\boldsymbol{b}_2 \cdot \boldsymbol{r}) + \frac{\boldsymbol{a}_1 \cdot \boldsymbol{b}_1 \times \boldsymbol{a}_3}{2\boldsymbol{a}_2 \cdot \boldsymbol{b}_1 \times \boldsymbol{a}_3}(\boldsymbol{b}_1 \cdot \boldsymbol{r})^2 + \frac{\boldsymbol{a}_2 \cdot \boldsymbol{b}_2 \times \boldsymbol{a}_3}{2\boldsymbol{a}_1 \cdot \boldsymbol{b}_2 \times \boldsymbol{a}_3}(\boldsymbol{b}_2 \cdot \boldsymbol{r})^2$$

- Corner charge

$$Q_{\mathrm{corner}} = \int_{\mathbb{R}^d} d^d r \rho_0(\boldsymbol{r}) Q_{123}(\boldsymbol{r})$$

$$c_{ij} \equiv -\frac{\boldsymbol{a}_i \cdot \boldsymbol{a}_j}{a_i^2} \qquad r_i \equiv \boldsymbol{b}_i \cdot \boldsymbol{r}$$

$$O_{123}(\boldsymbol{r}) = r_1 r_2 r_3 - \frac{1}{2}(c_{23} {r_3}^2 + c_{32} {r_2}^2) r_1 - \frac{1}{2}(c_{31} {r_1}^2 + c_{13} {r_3}^2) r_2 - \frac{1}{2}(c_{12} {r_2}^2 + c_{21} {r_1}^2) r_3$$
$$+ \frac{c_{23} {c_{31}}^2 + 2 c_{21} c_{31} + c_{32} {c_{21}}^2}{6(1 - c_{23} c_{32})} {r_1}^3 + \frac{c_{31} {c_{12}}^2 + 2 c_{32} c_{12} + c_{13} {c_{32}}^2}{6(1 - c_{31} c_{13})} {r_2}^3 + \frac{c_{12} {c_{23}}^2 + 2 c_{13} c_{23} + c_{21} {c_{13}}^2}{6(1 - c_{12} c_{21})} {r_3}^3$$

(Ambiguities in bulk multipole moment)

- $\rho_0(x)$ is not unique!

$$\rho^{(\mathrm{micro})}(\boldsymbol{r}) \equiv \langle \hat{\rho}(\boldsymbol{r}) \rangle = \sum_{n_i \in \mathbb{Z}} \rho_0(\boldsymbol{r} - \textstyle\sum_{i=1}^{d} n_i \boldsymbol{a}_i)$$

$$\begin{cases} \displaystyle\int_{\mathbb{R}^d} d^d r \rho_0(\boldsymbol{r}) = 0 \\ \rho_0(\boldsymbol{r}) \to 0 \quad \text{when } |\boldsymbol{x}| \gg a \end{cases}$$

$$\rho_0^{(\mathrm{el})}(x) = -\frac{ea}{L} \sum_{R} \sum_{n \in \mathrm{occ}} |w_{n,i}(R)|^2 \delta(x - R - x_i) \qquad w_{n,i}(R) \sim \int_0^{\frac{2\pi}{a}} \frac{dk}{2\pi} u_{nk,i} e^{ikR}$$

- Wannier center has only integer ambiguity
  → fractional part of polarization is well-defined.
  But spread of Wannier function is gauge-dependent.

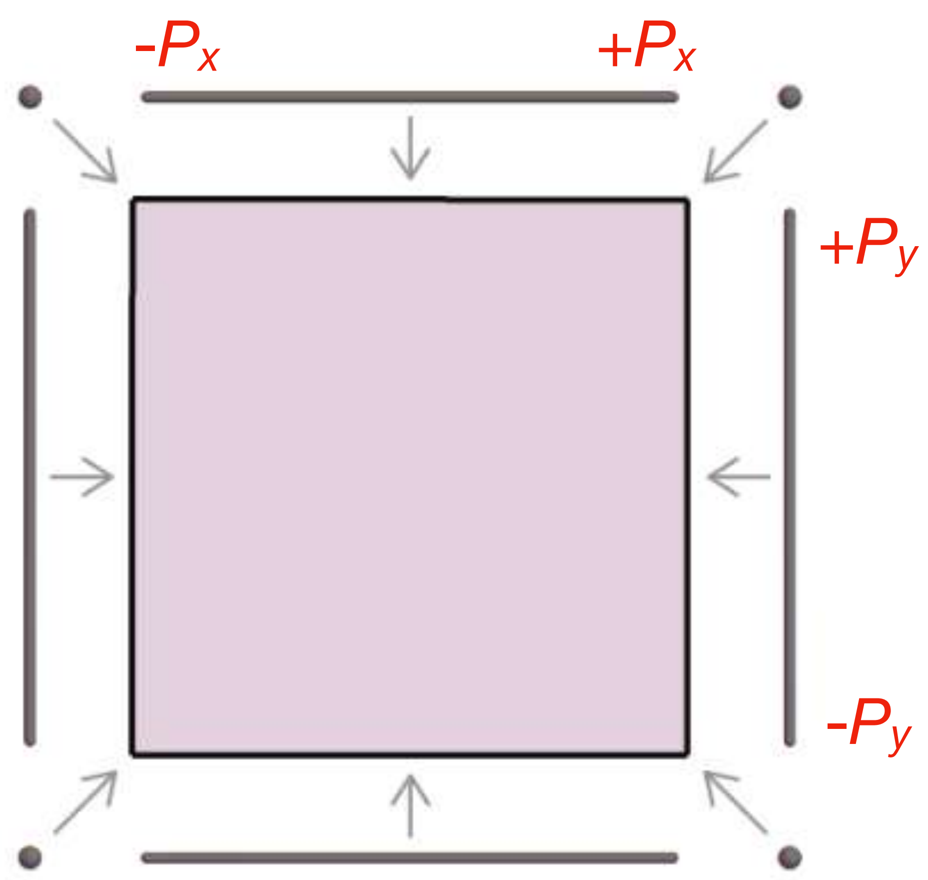
- Higher moments depend on the specific choice of $\rho_0(\boldsymbol{r})$

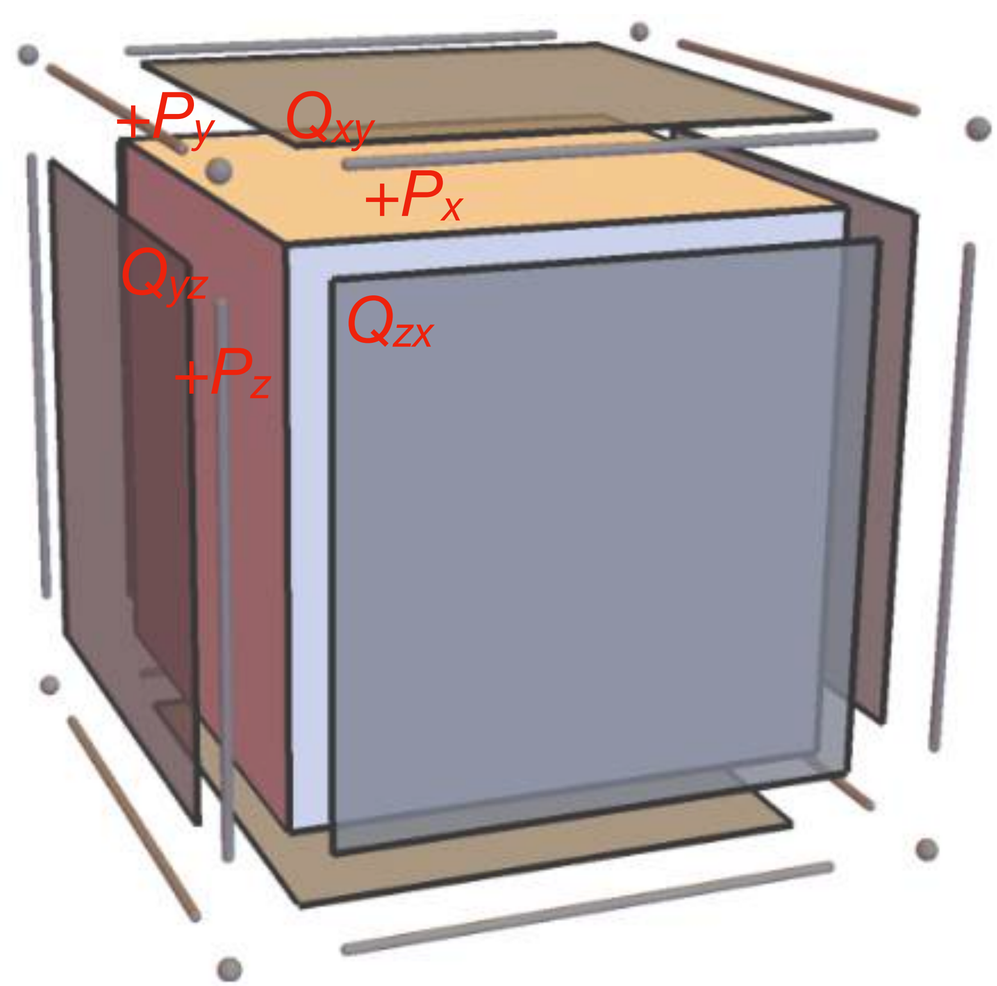
$$\int_{\mathbb{R}^d} d^d r \rho_0(\boldsymbol{r}) r_i \qquad \int_{\mathbb{R}^d} d^d r \rho_0(\boldsymbol{r}) r_i r_j \qquad \int_{\mathbb{R}^d} d^d r \rho_0(\boldsymbol{r}) r_i r_j r_k$$

Ambiguities in corner/hinger charge

$$Q_{\text{corner}} \to Q_{\text{corner}} + P_x + P_y$$

$$Q_{\text{corner}} \to Q_{\text{corner}} + P_x + P_y + P_z + Q_{xy} + \cdots$$





Corner charge not well-defined.

(Choice of termination & decoration)

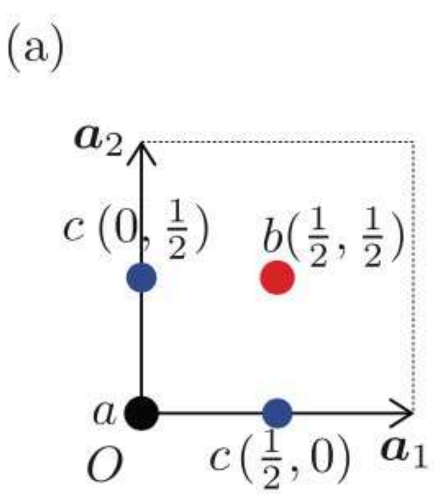
Point group symmetry is required!!

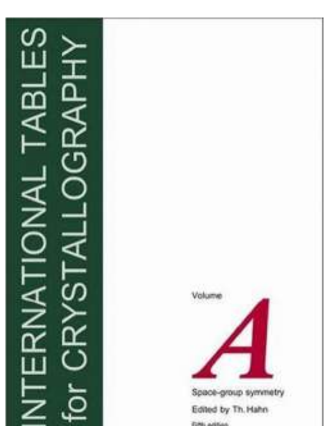
2D system under C_4 rotation

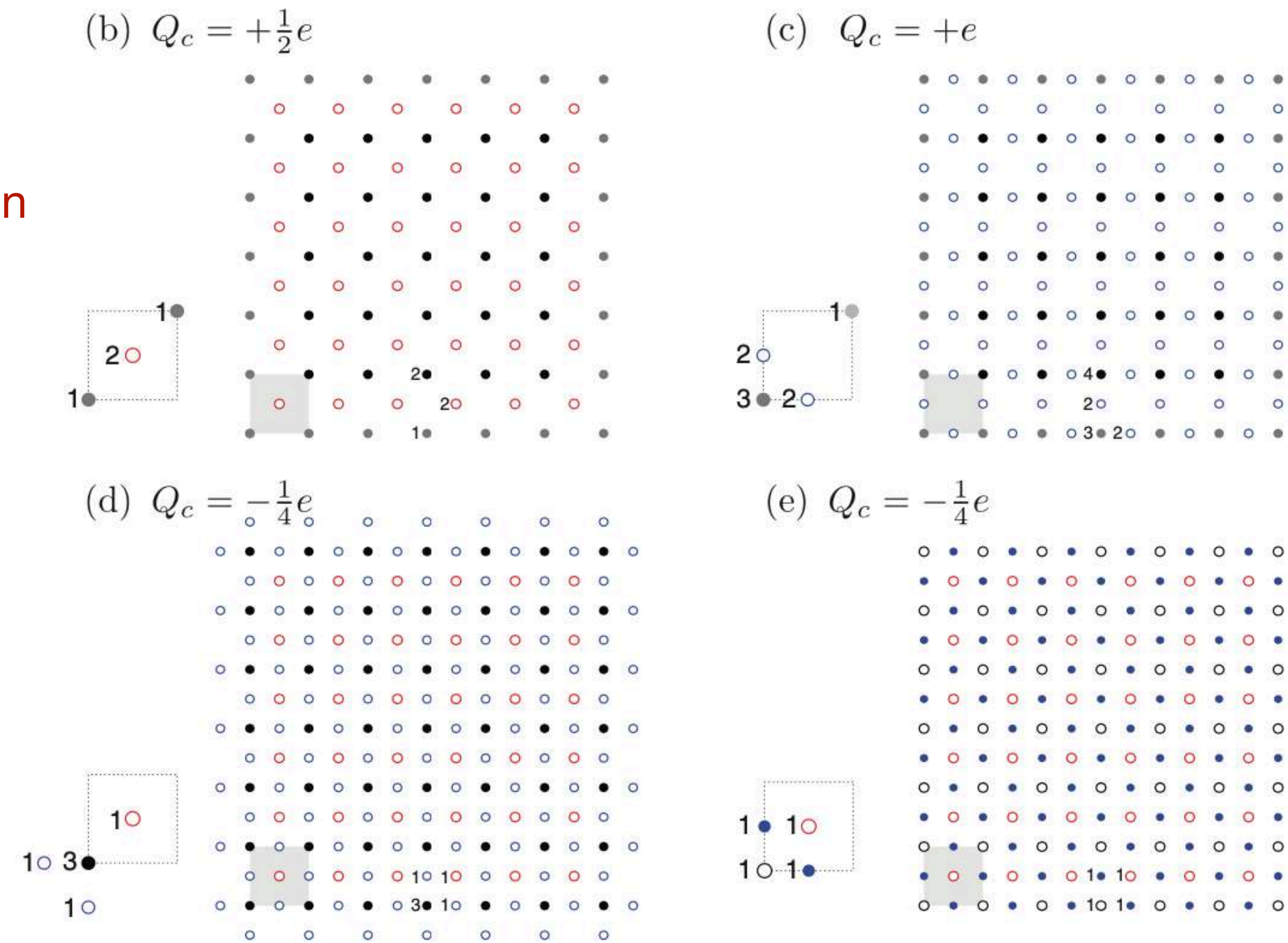
$$Q_{\mathrm{corner}} = \int_{\mathbb{R}^d} d^d r \rho_0(\boldsymbol{r}) Q_{12}(\boldsymbol{r}) = \frac{1}{4} q_a = \frac{1}{4} q_b \mod e$$

The U(1) charge on high-symmetry points

Classification of high-symmetry points: (special) Wyckoff position

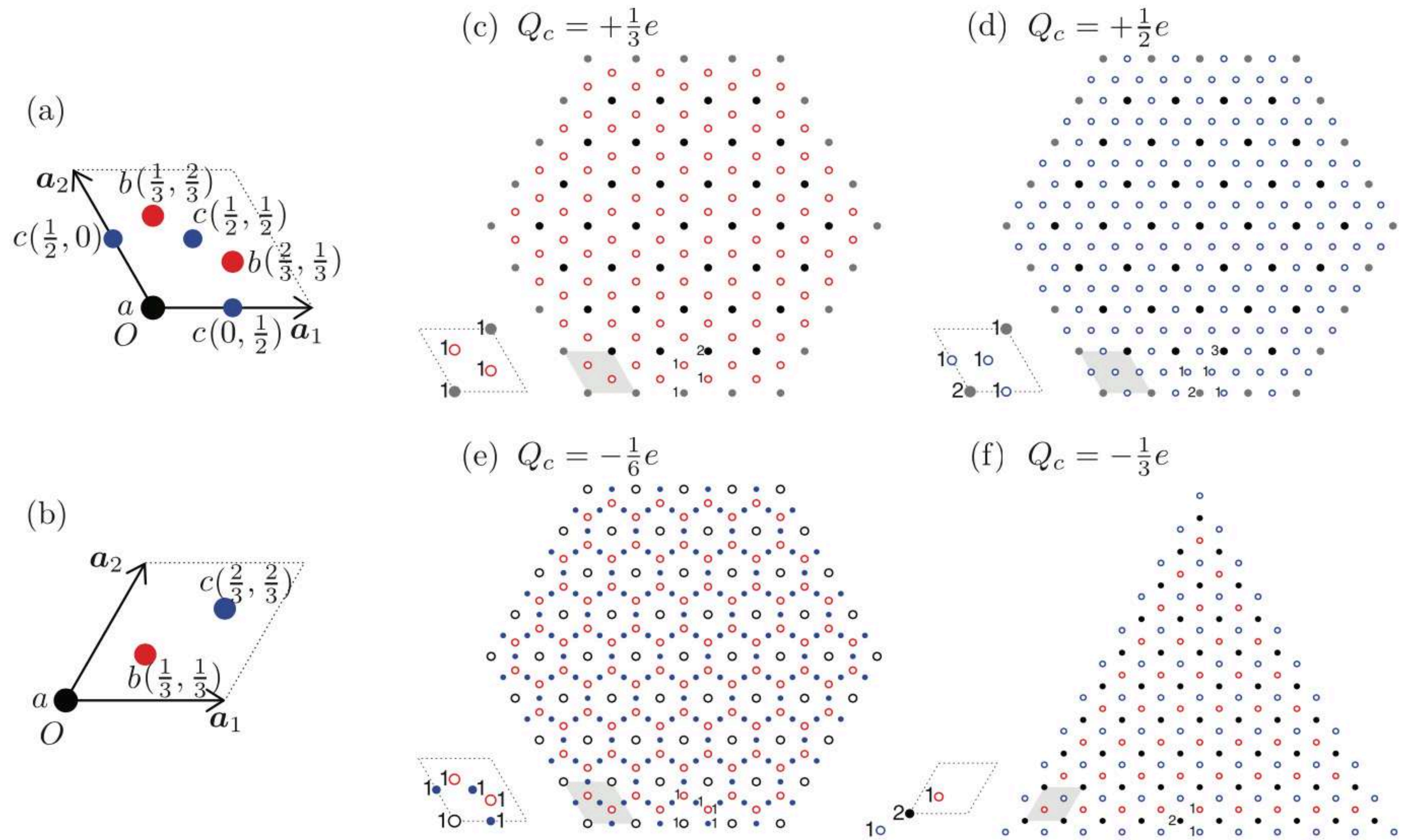






2D system under C_3 or C_6 rotation

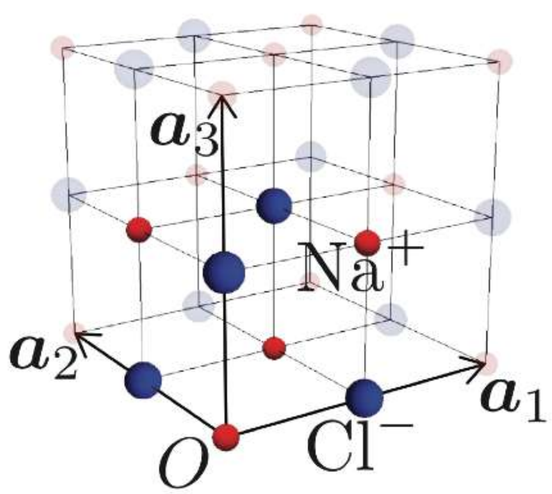
$$Q_{\text{corner}} = \int_{\mathbb{R}^d} d^d r \rho_0(\boldsymbol{r}) Q_{12}(\boldsymbol{r}) = \begin{cases} \frac{1}{6}q_a = \frac{2}{3}q_b + \frac{1}{2}q_c \mod e & (n=6) \\ \frac{1}{3}q_a = \frac{1}{3}q_b = \frac{1}{3}q_c \mod e & (n=3) \end{cases}$$

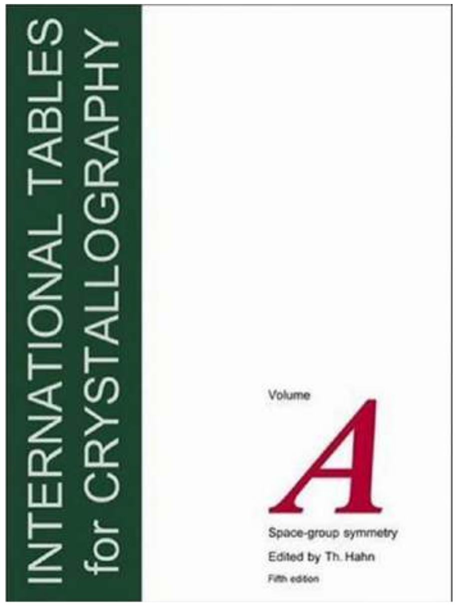


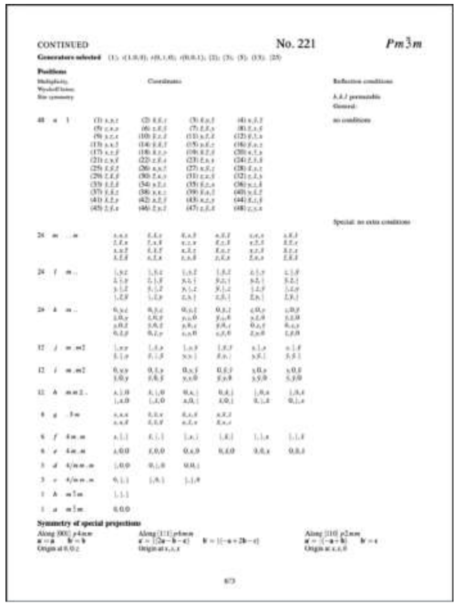
The U(1) charge Q mod ne at a C_n rotation axis is topological invariant.
Our results implies $Q_{\text{corner}} = Q/n \mod e$

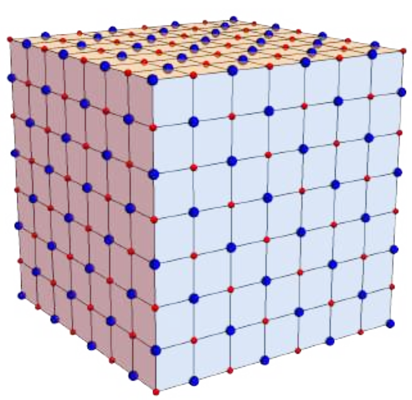
3D system under O_h symmetry

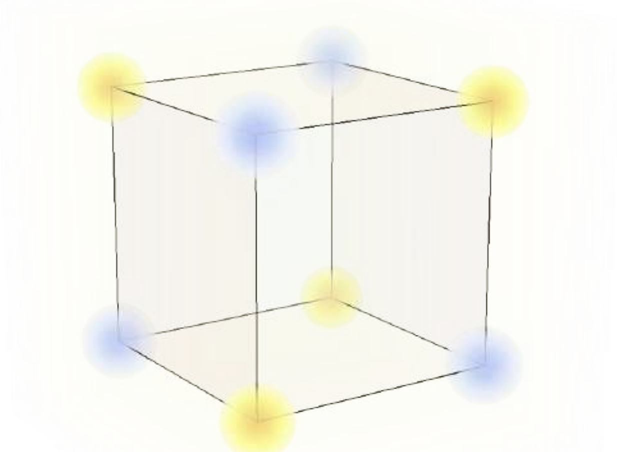
$$Q_{\text{corner}} = \int_{\mathbb{R}^d} d^d r \rho_0(\boldsymbol{r}) Q_{123}(\boldsymbol{r}) = \frac{1}{8} q_a = \frac{1}{8} q_b \mod \frac{1}{4} e$$











3	d	$4/m\,m\,.m$	$\frac{1}{2},0,0$	$0,\frac{1}{2},0$	$0,0,\frac{1}{2}$
3	c	$4/m\,m\,.m$	$0,\frac{1}{2},\frac{1}{2}$	$\frac{1}{2},0,\frac{1}{2}$	$\frac{1}{2},\frac{1}{2},0$
1	b	$m\bar{3}m$	$\frac{1}{2},\frac{1}{2},\frac{1}{2}$		
1	a	$m\bar{3}m$	$0,0,0$		

The U(1) charge Q mod $2e$ at a O_h center is topological invariant.
Our formula is $Q_{\text{corner}} = Q/8 \mod e/4$.

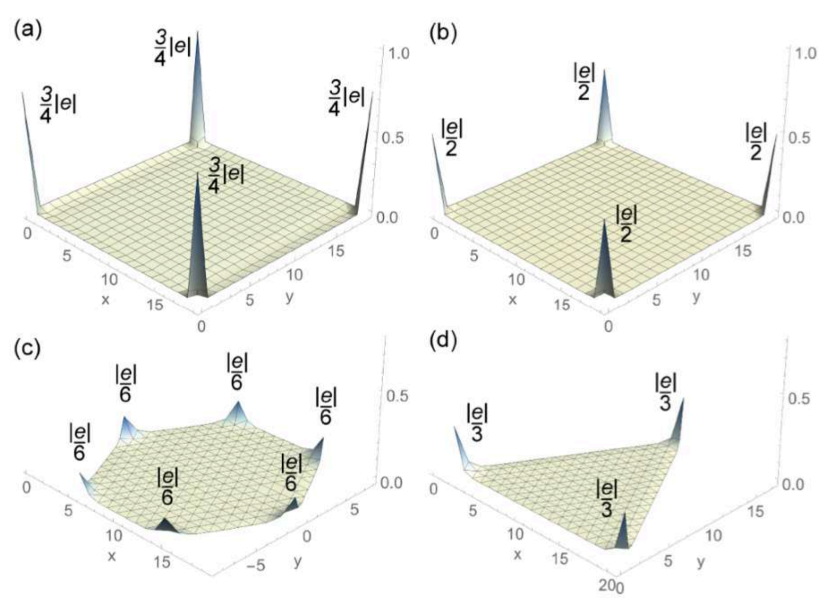
Filling anomaly

- Simple formula for the corner charge

$$Q_{\text{corner}} = Q_{\text{tot}} / N_{\text{corner}}$$

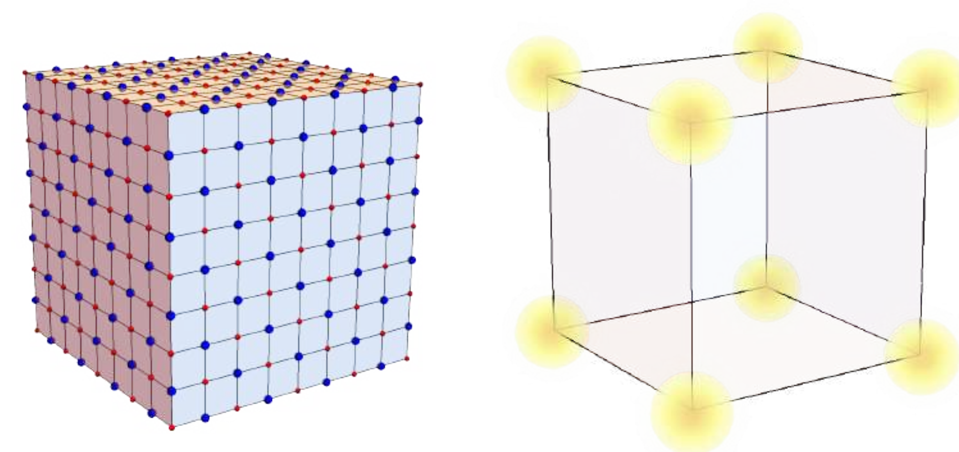
W. A. Benalcazar, T. Li, T. L. Hughes, PRB (2019)

Q_{tot} = The total U(1) charge in the system
N_{corner} = The number of point-group related corners



$$Q_{\text{tot}} = +e,\ Q_{\text{corner}} = \frac{1}{n}e \ \ (\text{mod } e)$$

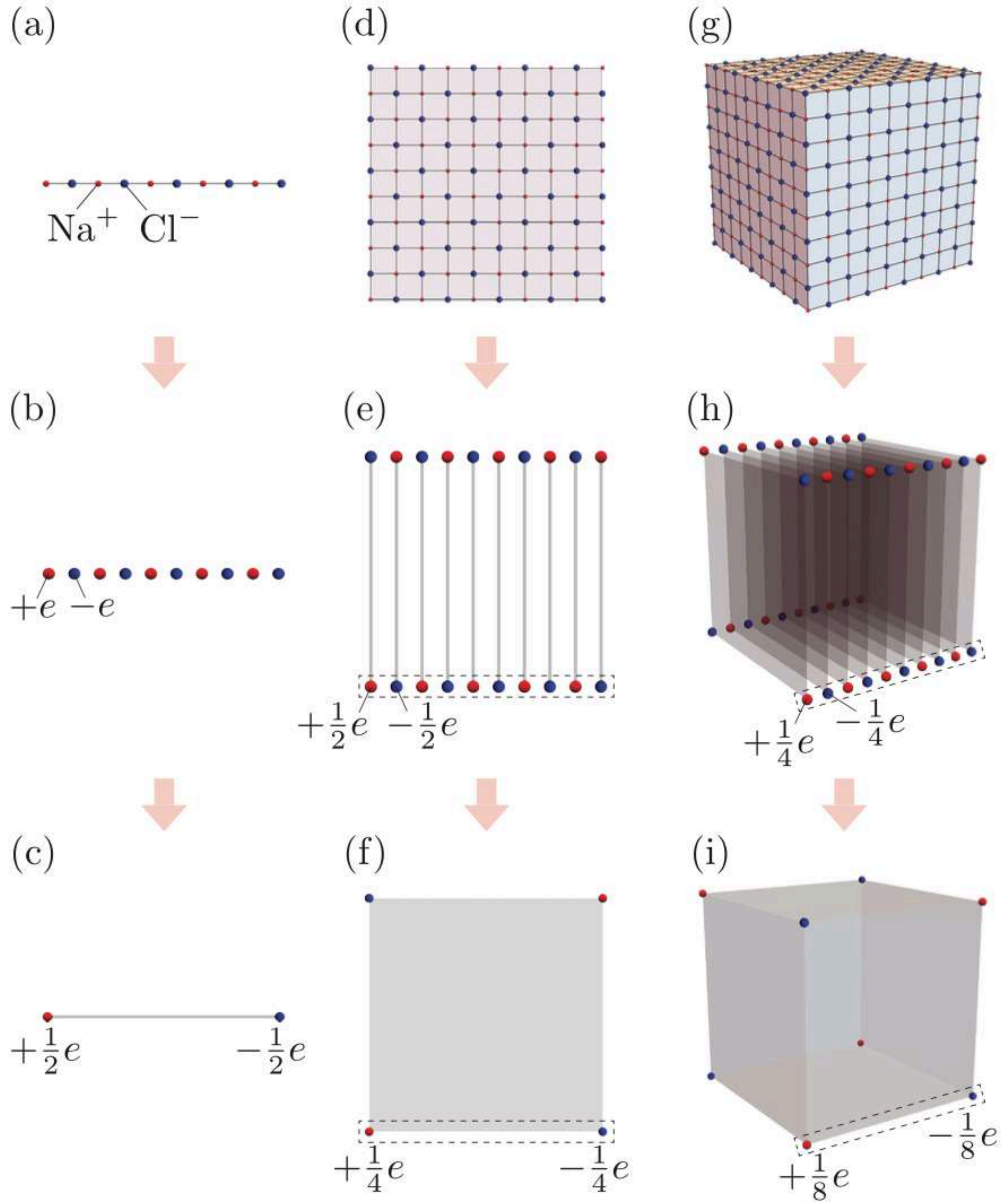
W. A. Benalcazar, T. Li, T. L. Hughes, PRB (2019)



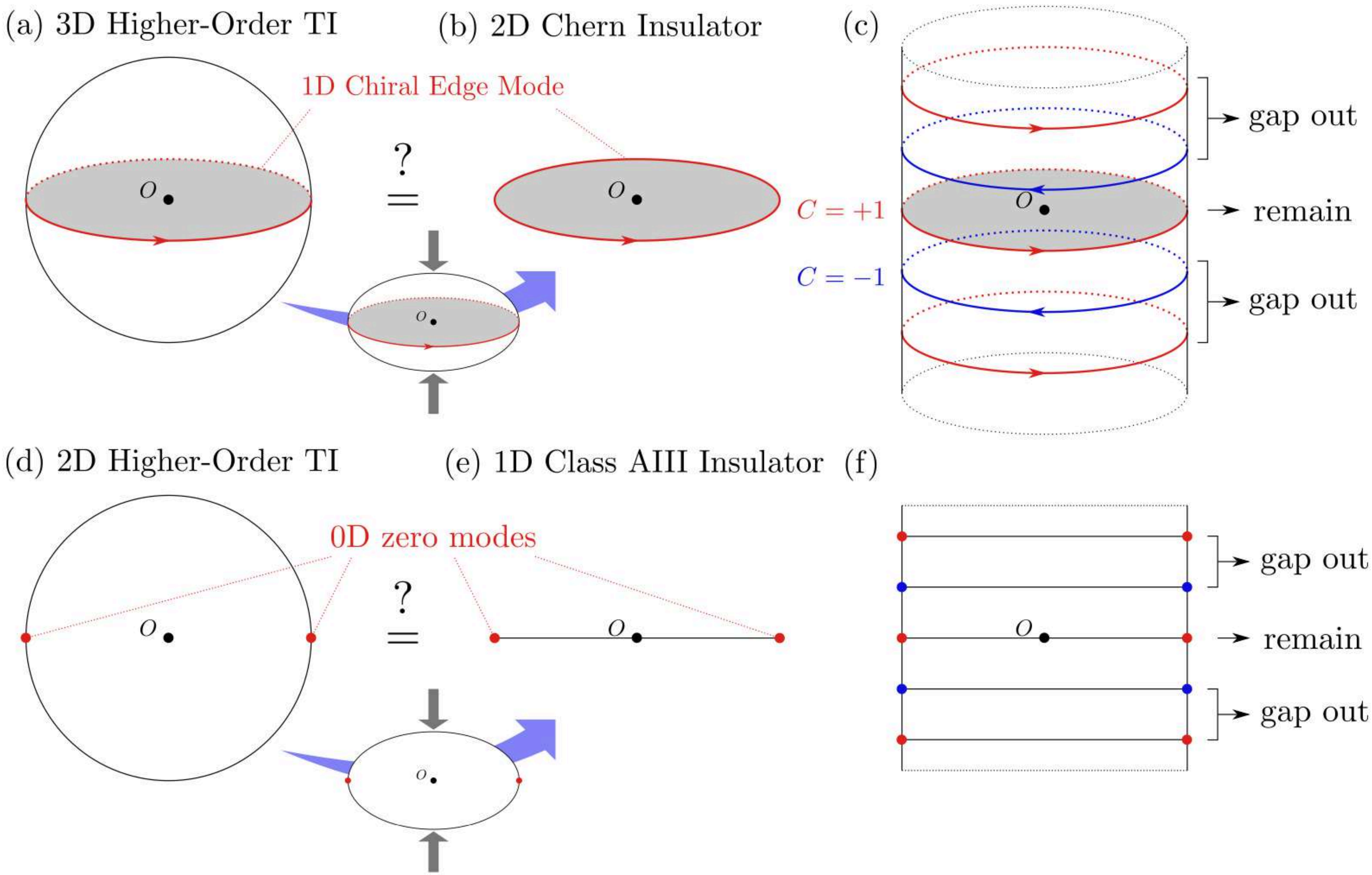
$$Q_{\text{tot}} = +e,\ Q_{\text{corner}} = \frac{1}{8}e \ \ (\text{mod } \frac{1}{4}e)$$

HW, S. Ono, PRB (2020)

Coupled-wire/layer argument



Similarity to HOTI



Matsugatani-Watanabe PRB (2018)

Traditional measurement of the bulk polarization

- Change a parameter and measure the electric current during the process.

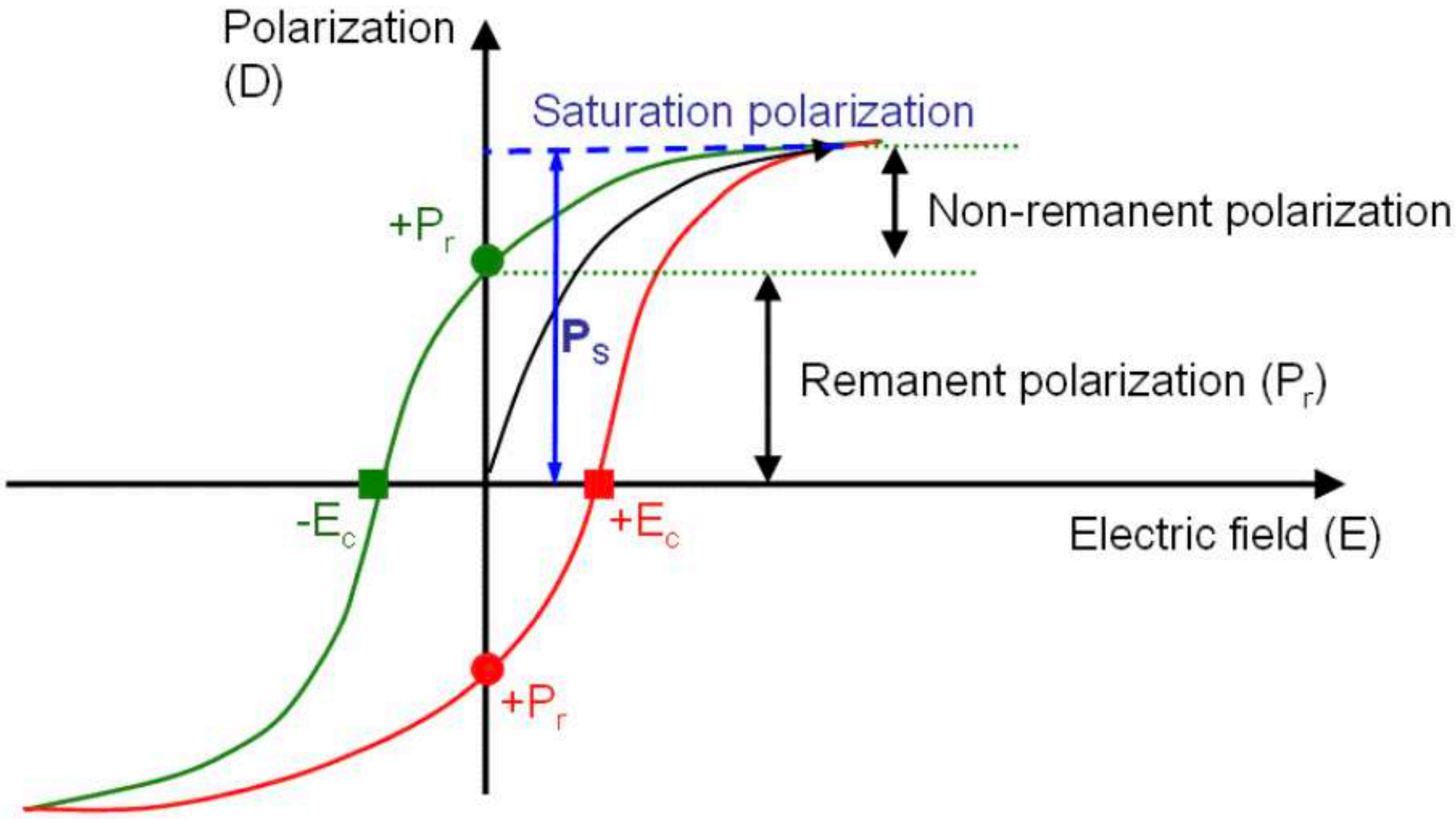
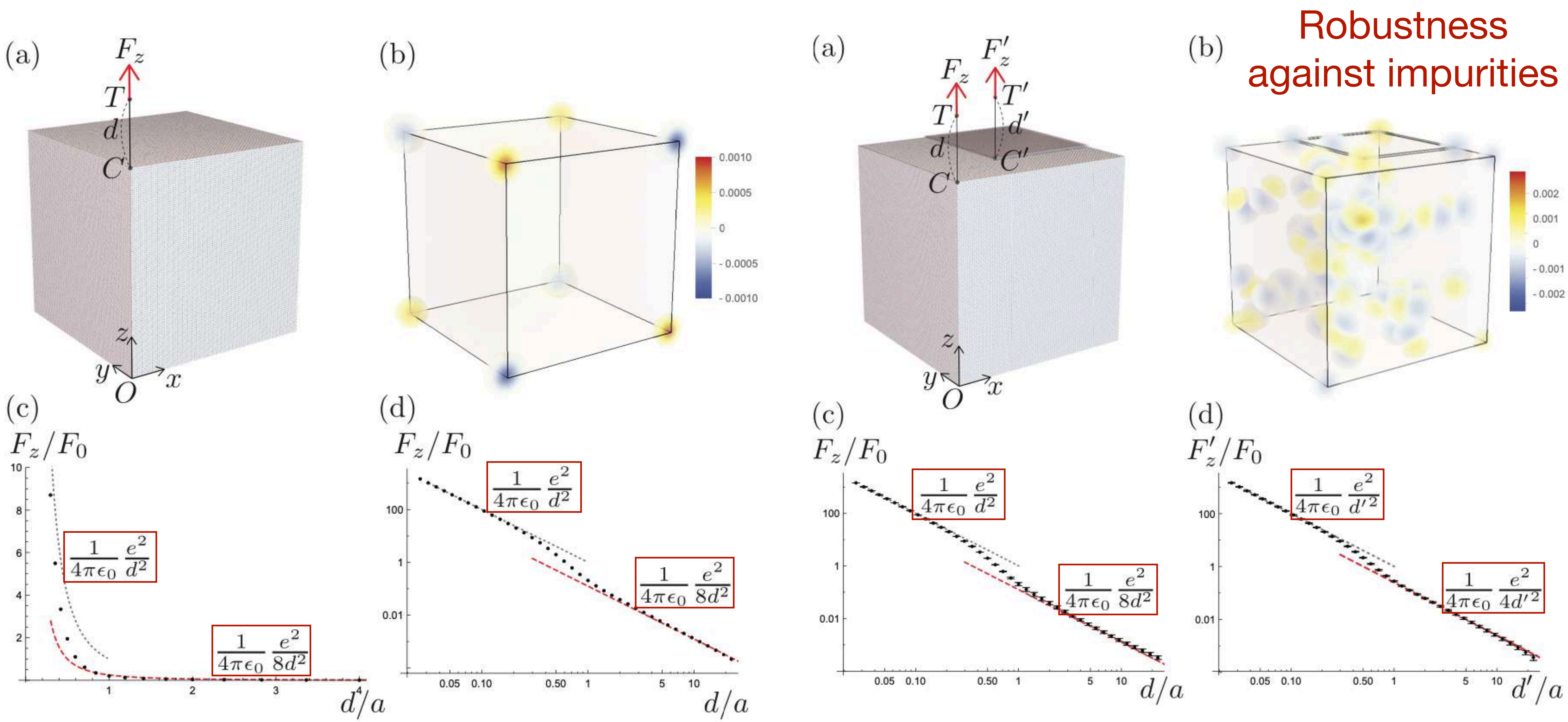


Figure from https://www.globalsino.com/EM/

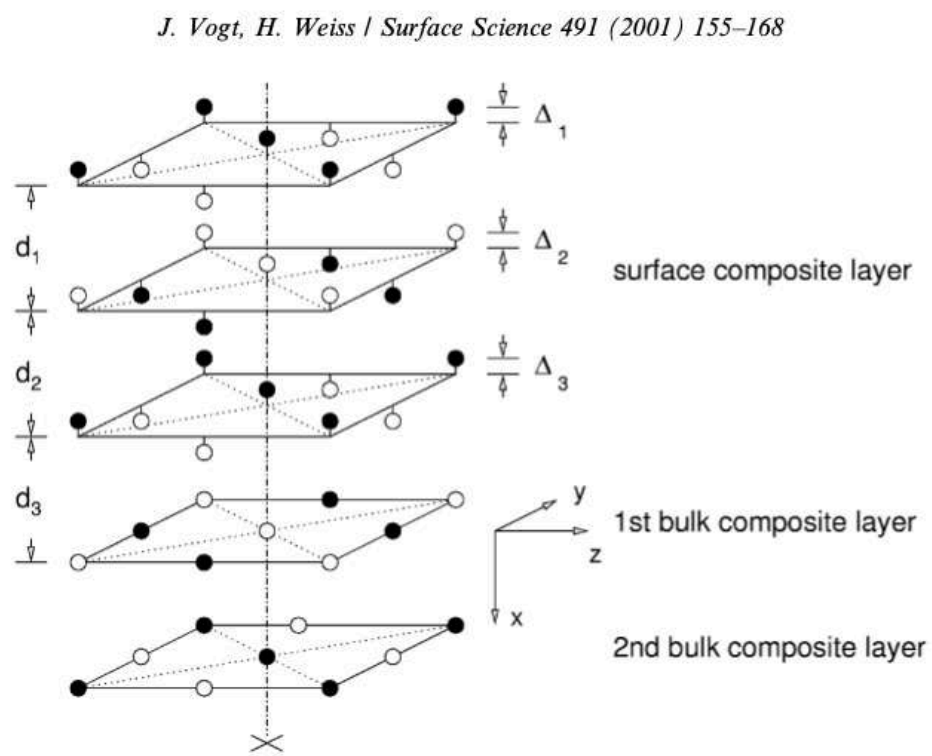
$$2P_x = \int_0^T dt J_x(t)$$

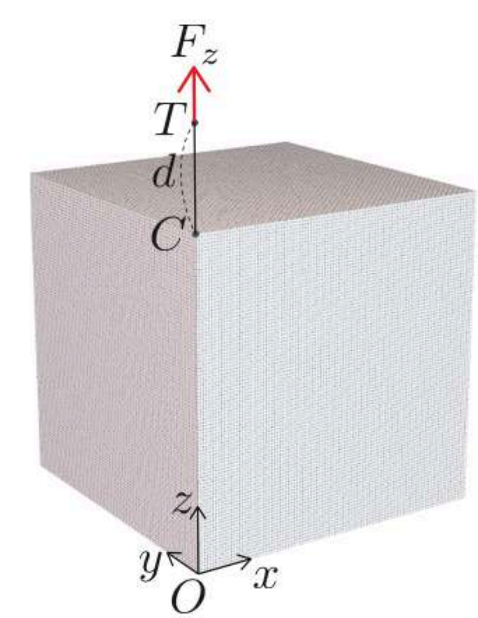
Possible direct measurement via atomic force microscope



$$F_0 \equiv \frac{e^2}{4\pi\epsilon_0 a^2} = 7.25 \times 10^{-10}\ \mathrm{kg\,m\,s^{-2}} = 725\ \mathrm{pN} \quad \text{for } a = 5.64\ \text{Å}$$

Corrections from surface dipoles & hinge polarizations





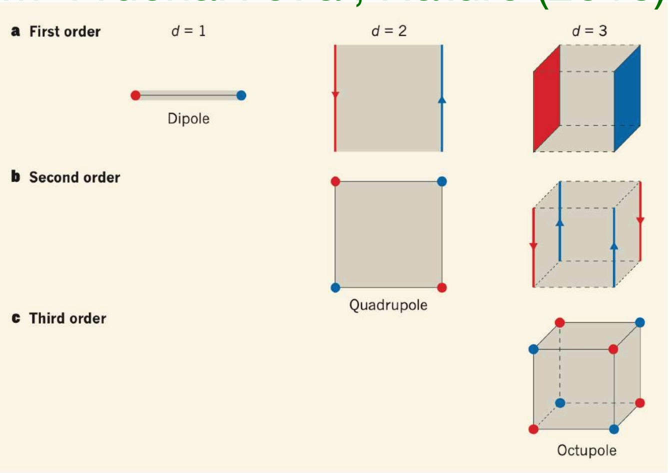
$$\boldsymbol{r}_0 = (0, 0, d)$$

$$\boldsymbol{E}(\boldsymbol{r}) = (0,0,1)\frac{Q_c}{d^2} + (-\tfrac{1}{8}, -\tfrac{1}{8}, \tfrac{1}{2})\frac{4p_h + 2p_s^a + p_s^c - 2q_s}{d^2} + O(d^{-3})$$

$$\boldsymbol{r}_0 = (d, d, d)/\sqrt{3}$$

$$\boldsymbol{E}(\boldsymbol{r}) = \frac{1}{\sqrt{3}}(1,1,1)\frac{Q_c}{d^2} + (1,1,1)\tfrac{3-\sqrt{3}}{4}\frac{4p_h + 2p_s^a + p_s^c - 2q_s}{d^2} + O(d^{-3})$$

M. Fruchart et al, Nature (2018)



Summary

- Topological vs Trivial

  - Higher-order *topological* insulators
  - Gapless *modes* on hinges / corners
  - Irremovable quantum entanglement

  - Higher-order *trivial* insulators
  - Fractional charges on hinges / corners
  - Connected to product state

- We bridged “multipole moments” and “filling anomaly”

Quadrupole moment

$$Q_{\mathrm{corner}} = q_{12}^{\mathrm{bulk}} = \int d^d r \rho_0(\boldsymbol{r}) \frac{xy}{a^2}$$

||

Filling anomaly

$$Q_{\mathrm{corner}} = \frac{1}{4} q_a = \frac{1}{4} q_b \mod e$$